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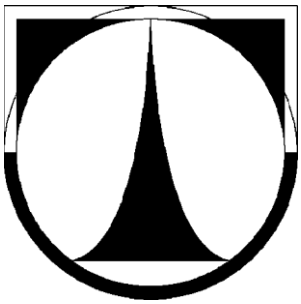

EXPERIMENTAL RESEARCH OF HYDROGEN FUELED ENGINE WITH HIGH PRESSURE DIRECT INJECTION

DOCTORAL WORK

2011 Ing. Manat Paengsai

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In Liberec, May 2011

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CONTENT

Commonly used symbols, subscripts and abbreviations

1. Symbols

Cp	Specific heat at constant pressure	kJ/kg.K
Cv	Specific heat at constant volume	kJ/kg.K
m	Mass	kg
n	Engine speed	RPM, min^{-1}
p_e	Mean effective pressure	MPa, bar
p_i	Mean indicated pressure	MPa, bar
p_{max}	Maximum pressure	MPa
Q	Total heat transfer	kJ
$\dot{\mathbf{Q}}$	Rate of heat transfer	kW
$\overline{\mathbf{R}}$	Universal gas constant	kJ/kmol.K
S	Stork of piston	m
t	Temperature	^oC
T	Temperature	K
V	Volume	m^3

2. Greek letters

α	Crank angle
Δ	Finite change in quantity
σ	Standard deviation
ε	Compression ratio
λ	Excess-air ratio
κ	Specific heat ratio

3. Subscripts

adv	Spark advance
avg	Average
c	Critical point
e	Effective
exh	Exhaust gaseous port
i	Indicated
inj	Injection
int	Intake port
ign, IGN	Ignition
t	Total

4. Abbreviations

ATDC	After bottom dead center
BTDC	Before top dead center
CA	Crank angle
EGR	Exhaust gas circulation
ER	Air equivalent ratio
CNG	Compressed natural gas
DOC	Duration of combustion
DI	Direct injection
CFD	Computational fluid dynamics
GH_2	Gaseous hydrogen
HHV	High heating value
HR	Heat release
Lamb	Lambda
LH_2	Liquid hydrogen
LHV	Low heating value
MPI	Multi point port injection
NA	Naturally aspirated engine
ROHR	Rate of heat release
RPM	Revolution per minute
SOI	Start of injection
TDC	Top dead center
TC	Turbocharger engine
VAR	Coefficient of variability
WOT	Wide open throttle or full load of engine

CHAPTER 1

1.1 Introduction

Fossil fuels, for example, petroleum, natural gas and coal, which meet most of the world's energy demand today, are being decreased quickly. Also, their combustion products are leading global problems, such as the greenhouse effect, ozone layer depletion, acid rains and pollution, which are creating great danger for our environment, and eventually, for the total life on our planet. Many engineers and scientists agree that the solution to all of these global problems would be to replace the existing fossil fuel system with the clean hydrogen energy system. Hydrogen is a very efficient and clean fuel. Its combustion will produce no greenhouse gases, no ozone layer depleting chemicals, and little or no acid rain ingredients and pollution. Hydrogen, produced from renewable energy (solar, wind, etc.) sources, would result in a permanent energy system which would never have to be changed.

Fossil fuels possess very useful properties not shared by non-conventional energy sources that have made them popular during the last century. Unfortunately, fossil fuels are not renewable. In addition, the pollutants emitted by fossil energy systems (e.g. CO, CO_2, SO_x, NO_x, unburned HC, radioactivity, heavy metals, ashes, etc.) are greater and more damaging than those that might be produced by a renewable based hydrogen energy system. Since the oil crisis in 1973, considerable progress has been made in the search for alternative energy sources. A long term goal of energy research has been seek for a method to produce hydrogen fuel economically by splitting water using sunlight as the primary energy source. Much fundamental research remains to be done.

Global utilization of fossil fuels for energy needs is rapidly resulting in critical environmental problems throughout the world. Energy, economic and political crises, as well as the health of humans, animals and plant life, are all critical concerns. There is an urgent need of implementing the hydrogen technology. A worldwide conversion from fossil fuels to hydrogen would eliminate many of the problems and their consequences. The production of hydrogen from non-polluting sources is the ideal way.

The economies of rich nations and the lifestyle of most of their residents depend on cars and light trucks. These vehicles contribute most of the carbon monoxide (CO), carbon dioxide (CO_2), volatile organic compounds (hydrocarbons, HC), and nitrogen oxides (NO_x) emitted in cities. It is clear that motor vehicles are important to the economy and lifestyle. Importance goes well beyond the direct consumer expenditures and indirect (support) expenditures, such as roads, suburbs, oil wells, refineries, and service stations.

Technology developments have created several challengers to the gasoline powered, internal combustion engine (ICE) vehicle. Short of some wonderful new technology emerging, the evolving gasoline fueled ICE will continue to be the choice of consumers and automakers. Even with regulatory pressure, it is doubtful that any technology would displace the gasoline fueled ICE—at least next 10 or 20 years. Perhaps, the only market

signal that would make a new technology more attractive would be a large increase in gasoline prices. The search for new technologies and fuels is driven by regulators, not the marketplace. The important gaps between the goals of society and those of individual manufacturers and drivers have been a major justification for government regulation. Regulators are mandating increasingly strict standards for emissions of air pollutants, the ability to use alternative fuels, and there is a warning of more strict fuel economy standards.

In addition to the concern for improving local air quality, regulators are concerned about lowering emissions, dependence on imported petroleum, and switching from petroleum to a more sustainable fuel. Regulators can penalize, or even prevent automakers from selling undesirable vehicles or fuel suppliers from selling undesirable fuels, but it is difficult to force consumers to buy what regulators consider to be desirable vehicles and fuels. Consumer appeal could lead to new propulsion systems or fuels, but consumers are generally satisfied with what they have now. For consumers to view new engines and fuels as more desirable, technology would have to produce superior performance and economy in these alternatives, or the current fuels would have to be seen as less desirable due, for example, to high greenhouse gas emissions.

Alternative fuels have the potential to solve many of the current social problems and concerns, from air pollution and global warming to other environmental improvements and sustainability issues. It is not a foregone conclusion that alternative fuels will throw aside advanced gasoline ICE vehicles soon.

Hydrogen has long been recognized as a fuel having some unique and highly desirable properties, for application as a fuel in engines. It is the only fuel that can be produced entirely from the plentiful renewable resource water, though through the expenditure of relatively much energy. Its combustion in oxygen produces uniquely only water but in air it also produces some oxides of nitrogen. These features make hydrogen an excellent fuel to potentially meet the ever increasingly strict environmental controls of exhaust emissions from combustion devices, including the reduction of green house gas emissions. Hydrogen as a renewable fuel resource can be produced through the expenditure of energy to replace increasingly the depleting sources of conventional fossil fuels. A brief statement and discussion of the positive features of hydrogen as a fuel and the associated limitations that are raising difficulties in its wide application as an engine fuel are both necessary and needed. Hydrogen gas has been in wide use as a fuel for quite a long time.

Additionally, enormous quantities of hydrogen are used increasingly as a raw material in a wide range of applications in the chemical industry, particularly in the upgrading of conventional fuel resources. The viability of hydrogen as a fuel in general and in engine applications in particular, is critically dependent on the effective, economic and satisfactory solution of a number of remaining key limiting problems. These limitations that hinder its widespread application as an engine fuel are primarily related to its production, storage, portability, transport and purity. These limitations can be considered to be far more serious than those facing the current and future applications of other fuels, including natural gas.

The use of hydrogen as an engine fuel has been attempted on very limited basis with varying degrees of success by numerous investigators over many decades and much information about their findings is available in the open literature. However, these reported performance data do not display consistent agreement between various investigators. There is also a tendency to focus on results obtained in specific engines and over narrowly changed operating conditions. Moreover, the increasingly greater emphasis being placed on the nature of emissions and efficiency considerations often makes much of the very early work fragmentary and mainly of historical value. Obviously, there is a need to be aware of what has been achieved in this field while focusing both on the attractive features as well as the potential limitations and associated drawbacks that need to be overcome for hydrogen to become a widely accepted and used fuel for engine applications. Also, there is a need to indicate practical steps for operating and design measures to be developed and incorporated for hydrogen to achieve its full potential as an attractive and superior engine fuel.

Production, Storage and Transportation of Hydrogen

1.2 Hydrogen Production Methods

Although hydrogen is the most plentiful element in the universe, making up about three quarters of all matter, free hydrogen is scarce. The atmosphere contains trace amounts of it (0.07%), and it is usually found in small amounts mixed with natural gas in crustal reservoirs. The Earth's surface contains about 0.14% hydrogen (the tenth most abundant element), most of which resides in chemical combination with oxygen as water. Hydrogen, therefore, must be produced. Logical sources of hydrogen are hydrocarbon (fossil) fuels (C_xH_y) and water (H_2O).

Presently, hydrogen is mostly being produced from fossil fuels (natural gas, oil, and coal). However, except for the space program, hydrogen is not being used directly as a fuel or as an energy carrier. It is being used in refineries to upgrade crude oil in the chemical industry to synthesize various chemical compounds (such as ammonia, methanol, etc.), and in metallurgical processes (as a reduction or protection gas). The total annual hydrogen production worldwide in 1996 was about 40 million tons [1]. Less than 10% of that amount was supplied by industrial gas companies; the rest was produced at consumer-owned and operated plants such as refineries and at ammonia and methanol production facilities.

A logical source for large-scale hydrogen production is water, which is abundant on Earth. Different methods of hydrogen production from water have been, or are being developed. They include electrolysis, thermochemical processes, photolysis, photoelectrochemical processes, and photocatalysis. Biomass is another important renewable resource for producing hydrogen. Some of these methods are described below (Table 1.2).

TABLE 1.2: Hydrogen Production Cost

Technology	Cost of H_2 ($/GJ)	Cost of H_2 ($/kg)
Direct biomass gasification	12.5-21.6	1.51-2.59
Steam reforming of bio-oil	10.3-19.9	1.24-2.38

Source: From Spath, P. L., Mann, M. K. and Amos, W. A. 2000. Update of Hydrogen from Biomass—Determination of the Delivered Cost of Hydrogen, NREL/MP-510-33112, National Renewable Energy Laboratory, Golden, CO; Craig, K. R. and Mann, M. K. 1996. Cost and Performance Analysis of Biomass Based Integrated Gasification Combined Cycle BIGCC Power Systems, NREL/TP-430-21657, National Renewable Energy Laboratory, Golden, CO.

Researchers are developing a wide range of processes for producing hydrogen economically and in an environmentally-friendly way. Most methods of producing hydrogen involve electrolysis - or splitting water (H_2O) into its component parts of hydrogen (H_2) and oxygen (O). The most common of process is currently steam reforming of natural gas, which converts methane (and other hydrocarbons in natural gas) into hydrogen and carbon monoxide by reaction with steam over a nickel catalyst. Other methods include:

- High-temperature steam electrolysis uses heat (approximately 1000°C) to provide some of the energy needed to split water, making the process more energy efficient.
- Thermo-chemical water splitting uses chemicals and heat in multiple steps to split water into its component parts.
- Photo-electrochemical systems use semi-conducting materials (like photovoltaic) to split water using only sunlight.
- Photo-biological systems use micro-organisms to split water using sunlight.
- Biological systems use microbes to break down a variety of biomass feedstock into hydrogen.
- Gasification using heat to break down biomass or coal into a gas from which pure hydrogen can be generated.

1.2.1 Electrolysis

Notably, electrolysis opens the door to producing hydrogen from any energy source capable of generating electricity, including fossil fuels, nuclear and renewable energies, such as solar, wind, or hydropower. But electrolysis requires substantial amounts of electricity, and is ultimately only as environmentally-friendly as the energy source used to generate the electricity. In terms of the ideal “hydrogen economy”, it is anticipated that the electricity required for the electrolysis process would come from renewable sources - because the production of hydrogen fuel that increases demand for fossil fuels promises no greenhouse gas mitigation

Currently, electrolysis provides only a small percentage of the world's hydrogen, most of which is supplied to industrial applications requiring small volumes of high purity hydrogen. Finally, it is expected that it will be decades before improvements in renewable energy technologies would yield generate electricity at a price which would enable hydrogen to compete with conventional forms of energy.

Electrolysis appears to be the only method developed to date that can be used for large-scale hydrogen production in a post-fossil-fuel age. Production of hydrogen by water electrolysis is a mature technology, based on a fundamentally simple process; it is very efficient, and does not involve moving parts.

The following reactions take place at the electrodes of an electrolysis cell filled with a suitable electrolyte (aqueous solution of KOH, NaOH, or NaCl) upon the application of a potential:

Cathode reaction :	$2H_2O(l) + 2e^- \rightarrow H_2(g) + 2OH^-(aq)$	(1.1)
Anode reaction :	$2\ OH^-(aq) \rightarrow \frac{1}{2}\ O_2(g) + H_2O(l)$	(1.2)
Overall cell reaction :	$H_2O(l) \rightarrow H_2(g) + O_2(g)$	(1.3)

The reversible decomposition potential ($E_{rev}= \Delta G/nF$) of the above reaction is 1.229 V at standard conditions. The total theoretical water decomposition potential is 1.480 V corresponding to hydrogen's enthalpy (because $\Delta H=\Delta G+T\Delta S$). Due to irreversible processes occurring at the anode and cathode, including the electrical resistance of the cell, the actual potentials are always higher, typically between 1.75 and 2.05 V. This corresponds to the efficiencies of 72 % to 82 %.

An electrolysis plant can operate over a wide range of capacity factors and is convenient for wide range of operating capacities, which makes this process interesting for coupling with renewable energy sources, particularly with photovoltaic (PV). Photovoltaic generate low-voltage direct current that is required for the electrolysis process. The performance of photovoltaic-electrolyzer systems has been studied extensively both in theory and in practice [1-4].

1.2.2 Thermochemical Processes

Thermochemical hydrogen production is a means of splitting water via a series of chemical reactions. All chemical intermediates are recycled internally within the process so that water is the only raw material and hydrogen and oxygen are the only products. The maximum temperature requirements for most thermochemical cycles lie within a temperature range of 650 -1100℃ [5], thus eliminating the use of lower-temperature heat sources. High-concentration solar collectors and nuclear reactors are the possible sources of heat for these cycles. According to Wendt [6] 2000-3000 different theoretical cycles have been proposed and evaluated.

Although theoretical efficiencies of hydrogen production by thermochemical cycles are as high as 50%, practical achieved efficiencies are extremely low. Material problems at the high temperatures have also hindered the development of efficient, scalable reactor concepts. The problems associated with the separation of hydrogen and oxygen, the depletion of intermediate products, and matching the reaction rates of the individual steps have further limited the practical implementation of thermochemical cycles. Thus far, only one cycle has been demonstrated on a bench scale and none of them have been demonstrated at a larger scale.

1.2.3 Biomass Hydrogen Production

Biomass represents a large potential feedstock resource for environmentally clean hydrogen production. It lends itself to both biological and thermal conversion processes. In the thermal path, hydrogen can be produced in two ways: direct gasification and pyrolysis to produce liquid bio-oil followed by steam reforming.

Direct gasification of biomass is in many ways similar to coal gasification. The process occurs broadly in three steps: biomass is first gasified (using steam or air) to produce an impure syngas mixture composed of hydrogen, CO, CO_2, CH_4, small amounts of higher hydrocarbons, tar, and water vapor. The gas may also contain particulate matter that is removed using cyclones and scrubbers. The particulate-free gas is compressed and then catalytically steam reformed to eliminate the tars and higher hydrocarbons.

This is followed by high and low temperature shift conversions to convert the CO to CO_2 and thereby produce additional hydrogen. Finally, the hydrogen is separated from other products by pressure swing adsorption (PSA) [7]. Figure 1.1 illustrates the sequence of processes. The main reactions taking place in biomass gasification are as follows:

$$\mathbf{CH_{1.5}O_{0.7} + 0.3H_2O \rightarrow CO + 1.05H_2 \quad \Delta H_R = +74.4 kJ/mol} \quad \text{(biomass gasification),} \tag{1.4}$$

$$\mathbf{CO + H_2O \rightarrow CO_2 + H_2 \quad \Delta H_R = -41.2 kJ/mol} \quad \text{(water-gas shift),} \tag{1.5}$$

Biomass typically contains about 6% hydrogen by weight. However, in presence of hydrogen-bearing species (steam), the hydrogen yield can be considerably improved above the 6% minimum [8]. Gasification temperatures encountered are typically in the range 600-850^{o}C, which is lower than many thermochemical water-splitting cycles, thereby making biomass gasification an attractive technology to produce hydrogen. Steam gasification of biomass is endothermic and the energy required for the process is supplied by burning part of the biomass feedstock or uncombusted char. Tars are polyaromatic hydrocarbons produced during gasification of biomass. Tars are undesirable coproducts as they clog filters, pipes, and valves and damage downstream equipments such as engines and turbines. Efforts are being made to minimize or reform the tars to additional product hydrogen [9].

Hydrogen can be alternately produced by reforming the biomass to a liquid bio-oil in a process called *pyrolysis*. Pyrolysis is an endothermic thermal decomposition of biomass carried out in an inert atmosphere at 450-550°C [10].

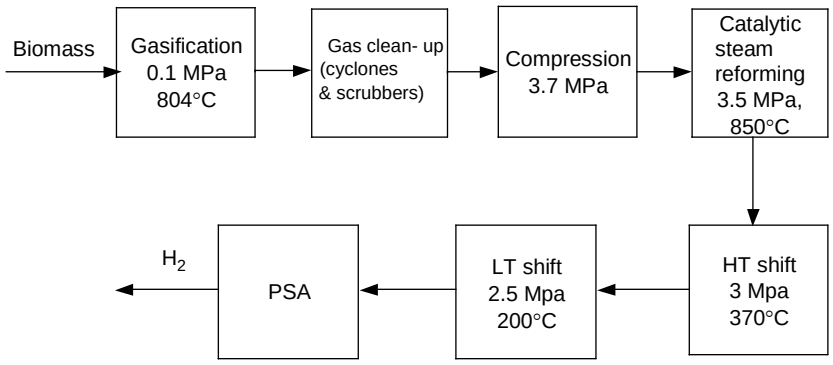


Figure 1.1 : Gasification followed by steam reforming. (From Spath, P. L., Mann, M. K. and Amos, W. A., 2000)

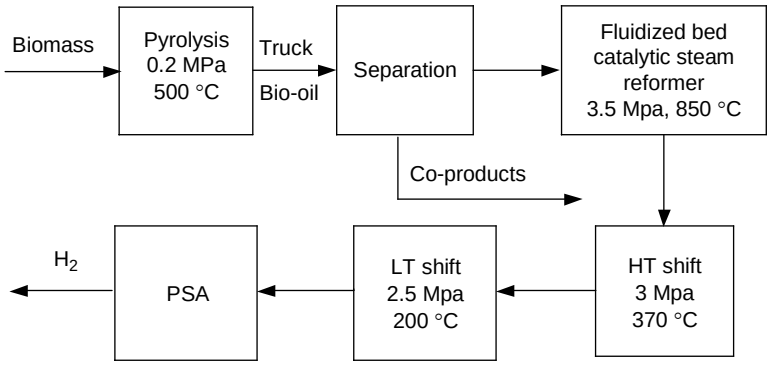


Figure 1.2: Pyrolysis followed by steam reforming. (From Spath, 2000. Update of hydrogen from biomass—Determination of the delivered cost of hydrogen, NREL/MP-510-33112, National Renewable Energy Laboratory, Golden, CO.)

The Bio-oil so produced is a liquid composed of 85% oxygenated organics and 15% water. The bio-oil is then steam-reformed in the presence of a nickel-based catalyst at 750 – 850^{o}C followed by shift conversion to convert CO to CO_2 which produces additional hydrogen [11]. Figure 1.2 illustrates the sequence of processes. The reactions can be written as:

$$\text{Biomass} \rightarrow \text{Bio - oil +char + gas} \quad \text{(pyrolysis)} \tag{1.6}$$

$$\text{Bio} - \text{oil} + H_2O \rightarrow CO + H_2 \quad \text{(reforming)} \tag{1.7}$$

$$CO + H_2O \rightarrow CO_2 + H_2 \quad \text{(shift)} \tag{1.8}$$

A number of research groups around the world are involved in research on hydrogen production from a variety of biomass resources, including wood, municipal solid waste, and residues from industries [12]. There are currently no commercial biomass gasification processes for hydrogen production but there are several demonstration plants of biomass gasifiers for producing electricity or chemicals [13].

However, an important factor that prohibits commercialization is the difficulty of transporting large amounts of low energy density biomass feed stocks over long distances. The cost associated with growing, harvesting, and transporting biomass may be up to 40% of the total biomass plant operating cost [14].

1.2.4 Biological Methods

Hydrogen may also be produced from biological processes involving organic compounds. The two fundamental ways of biological hydrogen production are: (1) fermentation of the bacteria, which is an anaerobic process that converts organic substances like, starch, cellobiose, sucrose, and xylose to H_2 and CO_2 without the need of sunlight and oxygen, and (2) biophotolysis, a process that uses microalgae cyanobacteria and green algae to produce hydrogen in the presence of sunlight and water. Both of these processes are being researched. However, the efficiencies of these processes are so low that they are not an option in the near term.

Thermo-chemical processes can also be applied to bio-resources such as agricultural residues and wastes or biomass specifically grown as an energy crop to produce hydrogen through pyrolysis and gasification. This process generates a carbon-rich synthetic gas that can be reformed into hydrogen using thermal processing techniques similar to fossil fuels reformation. Gasification technology has been under intensive development over the last two decades; a number of demonstration facilities have been tested and many units are in operation. Until recently, biomass gasification has been employed to produce electricity or heat.

1.2.5 Hydrogen from Fossil Fuels

Hydrogen gas can be derived from hydrogen-rich fossil fuels through a variety of processes. Currently, the most prevalent and least-expensive way to produce hydrogen is to derive it from natural gas through a process called steam reformation.

Hydrogen can also be produced from coal, through gasification. Fossil fuels can indirectly be used to produce hydrogen when they are used to generate electricity used in the electrolysis of water. Since this practice includes emissions related to the fossil fuel consumption. The current hydrogen world production rounds to some 40 million ton a year. Most of this hydrogen is produced from steam reforming of natural gas and used in refinery as a process gas, in chemical industry and in metal manufacturing.

a) Steam reformation

Steam reforming uses thermal energy to separate hydrogen from the carbon component of hydrogen rich fuels by reacting them with steam on catalytic surfaces. Although steam reformation is a relatively efficient and inexpensive process, this depends upon the fluctuating price of natural gas (or other feedstock fuel). In terms of the environment, steam reformation generates CO_2 emissions, both as a by-product of the reformation process and during fossil fuel production and transportation (upstream) phases. As such, research typically focuses on how to make the process more efficient and utilizing waste heat for other purposes.

b) Gasification of coal

Gasification of coal may be the oldest method of producing hydrogen. This technique was the source of the "city gas" that was originally supplied to many cities in Europe and Australia before natural gas became available. This gas contains up to 60% hydrogen, but also large amounts of CO. To make it, the coal is typically heated to 900°C where it turns into a gaseous form; it is then mixed with steam and in the presence of a catalyst a mixture of H_2, CO and CO_2 is produced. In addition, sulphur and nitrogen compounds are released during the process, which like the CO and CO_2, must be handled in an environmentally-friendly way.

1.2.6 Hydrogen production from nuclear energy

Hydrogen production holds renewed promise for nuclear energy, as nuclear-based hydrogen production can provide an essentially carbon emissions-free source of hydrogen, significantly reduce dependence on fossil fuels, and open a new area of application for nuclear energy that may eventually exceed the use of nuclear power for electricity.

Three approaches are being investigated: The first is to use nuclear heat to assist with the energy needs required by steam reformation for producing hydrogen from fossil fuels (e.g., natural gas). Secondly, several direct thermo-chemical processes are being developed for producing hydrogen from water. For economic production, high temperatures are required to ensure rapid throughput and high conversion efficiencies. A third way, of course, is to use nuclear power to supply electricity for electrolysis.

1.3 The concerning of hydrogen storage

Cost is the biggest impediment in using hydrogen more widely as a fuel. Many expensive changes must be made in the infrastructure to accommodate hydrogen. As an example, electricity is required by many hydrogen production methods, which makes hydrogen more expensive than the fuels it would replace. Another impediment on using hydrogen is its storage, which is the following step to the production.

The techniques available for storing hydrogen can be divided in two different types: the first type being physical and the second one chemical. Physical means concern the gaseous and liquid state of hydrogen, and the chemical one, can be either reversible or irreversible. The reversible chemical storage of hydrogen is done with metal hydrides or to hydrogen adsorption on carbon materials and the irreversible chemical storage is done with some complex hydrides.

Two physical storage techniques - hydrogen compression and hydrogen liquefaction - and one chemical storage technique - hydrogen chemisorption on metal hydrides - will be explained in the following paragraphs.

1.3.1 Compressed hydrogen

Hydrogen can be stored as a compressed gas in storage tanks, and new materials allow storage tanks to keep hydrogen at extremely high pressures. Considering that hydrogen has an extremely low critical temperature, unless it is brought to cryogenic temperatures, hydrogen remains a gas whatever the pressure applied at temperatures down to -239.8°C.

In the case of the compression of hydrogen in a tank, the amount of hydrogen stored in the tank is determined by a gravimetric percentage. This gravimetric percentage is defined as the mass of hydrogen compressed in the tank divided by the mass of the tank and of the hydrogen present in the tank.

Types of vessels for compression

Two major advances that have been done in the tanks for the compression of hydrogen are the new materials that allow higher hydrogen pressures and the evolution of the concept of the tank concept.

The idea was to place a double envelope on the cylinders, the first liner for the non-permeability of the cylinder and the second reinforcement - the over-wrapping - for the strength to weight ratio [15]. The initial reinforcement was only on the cylindrical part with a hoop wrap (type II tank), but this reinforcement was quickly evolved to a complete wrapping of the cylinder, a fully wrap (type III tank), until the final tanks have been developed where the liner, in the type IV tank, is a non-metal liner. The four different types are shown on the Figure 1.3 below:

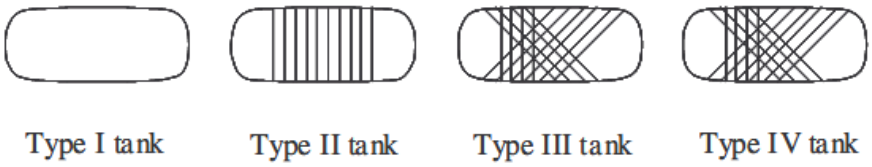


Figure 1.3: Four different types of tanks

The four different types of tanks actually developed:

- Type I - all metal cylinders
- Type II - metal liner hoop wrapped with resin impregnated continuous filament
- Type III - metal liner fully wrapped with resin impregnated continuous filament
- Type IV - non-metal liner wrapped with resin impregnated continuous filament

The mass per unit volume since the type I cylinder has diminished by 75%, decreasing from 1.16 kg/L for a type I steel cylinder to 0.30 kg/L for a plastic/carbon type IV cylinder. In terms of storage gravimetric capacities of hydrogen, the type I cylinder is around 2 to 3%, the type III cylinder is around 5% and the storage capacity of the type IV cylinder should reach up to 10% [16].

Currently, the most preferred lightweight composite cylinder on the market is the DyneCell cylinder, developed and manufactured by Dynetek industries [17]. It is a lightweight cylinder designed for the storage of compressed gases such as hydrogen and natural gas and is built from a seamless 'thin wall' aluminum liner with a full carbon fibre overwrap, hence a type three cylinder. The liner technology guarantees ultra-light weights, high storage capacities and non-permeability while the carbon fiber overwrapping insures the corrosion resistance and maximizes the strength to weight ratio and operation performance under the harshest environments.

1.3.2 Liquefied hydrogen (LH_2)

An alternative to the storage of hydrogen through compression is the storage of hydrogen in its liquid state through liquefaction. Condensing hydrogen gas into the more dense liquid form enables a larger quantity of hydrogen to be stored and transported. As a reminder, the density of hydrogen as a gas is 0.09 $kg.m^{-3}$ (at room temperature and atmospheric pressure) and as a liquid 70.8 $kg.m^{-3}$ and the critical point of hydrogen is at a temperature of T_c = -239.8°C and a pressure of P_c = 13 bars. In order to liquefy the hydrogen gas it is essential to decrease the temperature below that critical temperature. Compressing the gas at a temperature above the critical temperature will not liquefy it, whatever the pressure applied.

a) The liquefaction process

Prior to the liquefaction process, the gaseous hydrogen used is purified, because at the boiling temperature of liquid hydrogen, all gases are solid. This enables to obtain very pure hydrogen. The hydrogen liquefaction consists of a heat exchange process with three essential steps:

- The pre-cooling stage from 27°C down to -193°C

This enables to bring the gaseous hydrogen below the inversion temperature of Joule-Thomson, temperature above which a gas expansion leads to the heating of the gas. This is done thanks to a mechanical refrigeration system from 27°C down to -38°C, and by a nitrogen cycle (vaporization of liquid nitrogen) from -38°C to -193°C.

- The final cooling and liquefaction from -193°C down to -253°C

This stage is realized by using either a helium cycle (Brayton cycle). These cycles consists in a succession of compression cycles with one or more gas compressors followed by some gas expansions (with heat extraction) through one or more turbines. The gas is cooled down during these cycles to -253°C, and is subject to a Joule-Thomson expansion through a valve. At the end of this transformation, liquid hydrogen is obtained.

- The conversion of ortho to para-hydrogen

It is catalyzed by hydroxide iron $Fe(OH)_3$ during liquefaction as it is a low exothermic reaction. Indeed at -253°C and 1 bar, the conversion enthalpy (520 kJ/kg), is greater than the vaporization enthalpy of liquid hydrogen (448 kJ/kg). If the conversion does not occur prior to the storage, it can lead to the vaporization of a large amount of the liquid hydrogen during the storage [18].

The liquefaction of hydrogen requires around 10 kWh/kg for industrial processes, which represents about 30 to 40% of the energy contained in hydrogen if one refers to the net calorific value of 33 kWh/kg. This makes the process a very costly one, and constitutes one of the major inconveniences on the use of liquid hydrogen for specific applications such as the automobile.

b) The cylinders used for LH_2

Once the hydrogen is liquefied one should store it in a super-insulated tank. These tanks are generally either cylindrical or spherical in order to minimize the surface to volume ratio, which limits the heat exchanges through the surface.

Whatever the level of isolation obtained for these tanks, there is always some heat exchange, which can be limited to less than 1 W for certain tanks. The vaporization heat of LH_2 being very low there is always some liquid hydrogen evaporation in the tank. The accumulation of the vapors in the tank leads to an increase in the pressure inside the tank, which has to be boiled off. In case of prolonged storage, it is essential to evacuate the gaseous hydrogen in order to maintain the pressure below the maximal critical pressure, generally 8 bars.

A typical tank for liquid hydrogen consists in a volume with a double envelope in between which the insulating materials are placed as show in figure 1.4.

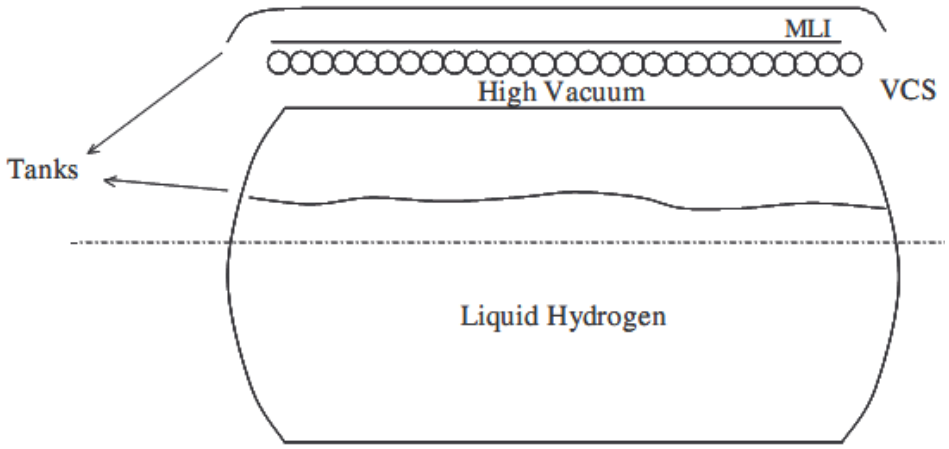


Figure 1.4: Schematic representation of a liquid hydrogen tank [18]

The principle is based on minimizing the heat transfer between the two envelopes and the thermal bridges between the internal and external surfaces. The space between the shells is under vacuum in order to minimize the conduction and convection heat transfers. Hydrogen being a very small molecule it tends to diffuse out the internal shell to the annular space. In order to maintain the vacuum, it is required to place an adsorbent.

An insulating material is placed in between the shells and reduces the heat conduction. This material forms the multilayer insulation (MLI) and is placed under vacuum. Moreover, to increase the insulation, a vapor cooled shield (VCS) is placed in the double envelope. This shield is metallic and is cooled by the circulation of a cold fluid (nitrogen).

The insulating material should be the most performing one at low temperatures on the basis of the thermal conductivity. The materials used are Perlite and multi-layer vacuum super insulation (MLVSI). This material consists in a series of reflecting screens of weak emissivity separated by layers of low conducting materials. The thickness of this super-insulation is around 2 to 5 cm with an optimal of 15 to 40 layers per cm thickness.

c) Actors and applications

Three major different types of applications are possible for liquid hydrogen: stationary, spatial and automotive applications. Stationary applications consist in storing the liquid hydrogen close to sites where liquid hydrogen will be required and more specifically on spatial sites. The largest capacities are in the spatial industry due to the high demand of the space shuttles.

A few examples of the use of liquid hydrogen for automotive applications exist, such as BMW in 2001 with a tank of 120 L of LH_2, Renault in the FEVER project with a tank reservoir of 120 L in 1997, Daimler Chrysler in 1999 with the NECAR 4 and 70.5 L of LH_2 in a 100 L tank or Ford with 68 L of LH_2 in 2001. The classical capacities used for the most recent demonstrations are comprised between 63 and 120 L of LH_2, meaning between 4.5 and 8.5 kg of hydrogen.

The advantages of this storage technique is its high density and the low pressure storage, but the drawbacks are still important due to the energy requirements for liquefaction, the cost, the complexity of the tank fabrication and the losses due to evaporation. The main directives for research and development on liquid hydrogen storage are on the optimization of the insulation system, new geometries for the tanks and reducing the weight and cost of the tank.

1.4 Metal hydrides

Another method of storing hydrogen is to trap it in a metal hydride. When certain metal alloys are exposed to hydrogen gas, a chemical reaction occurs between the alloy and the hydrogen. The alloy absorbs large quantities of hydrogen and forms a solid metal hydrogen compound. The hydrogen can be released (desorbed) as a gas and the alloy returns to its original state.

The hydriding and dehydriding of metals M by both direct dissociative chemisorption of hydrogen gas and electrochemical splitting of H_2O are simple

$$\mathbf{M + x.H_2O + x.e^- \leftrightarrow MH_x + x.OH^-} \tag{1.9}$$

$$\mathbf{M + \frac{x}{2} H_2 \leftrightarrow MH_x} \tag{1.10}$$

A common method used to characterize metal hydrides is by using a graph in which the hydrogen equilibrium pressure is plotted versus the hydrogen to metal ratio at a constant temperature. These curves are commonly called the pressure composition isotherms and give the equilibrium pressure-composition at a given temperature.

1.5 Carbon materials used for hydrogen storage

The carbon materials actually tested for hydrogen storage are mainly activated carbons, graphite nanofibre, carbon nanotubes and fullerenes. These materials exhibit interesting properties for hydrogen storage either for hydrogen adsorption (graphite nanofibres, activated carbon and nanotubes) or through chemical storage. Prior to investigating the recent research done on the hydrogen storage in these carbon materials, the following paragraph will present these various families of carbon materials that are interesting for hydrogen storage.

Graphite and diamond were initially the two only forms of crystalline carbon until the fullerene was discovered. The phase diagram below shows that the stable phase for carbon is graphite at low and medium pressure and temperature, whereas diamond is the stable form at high pressure due to its higher density [19].

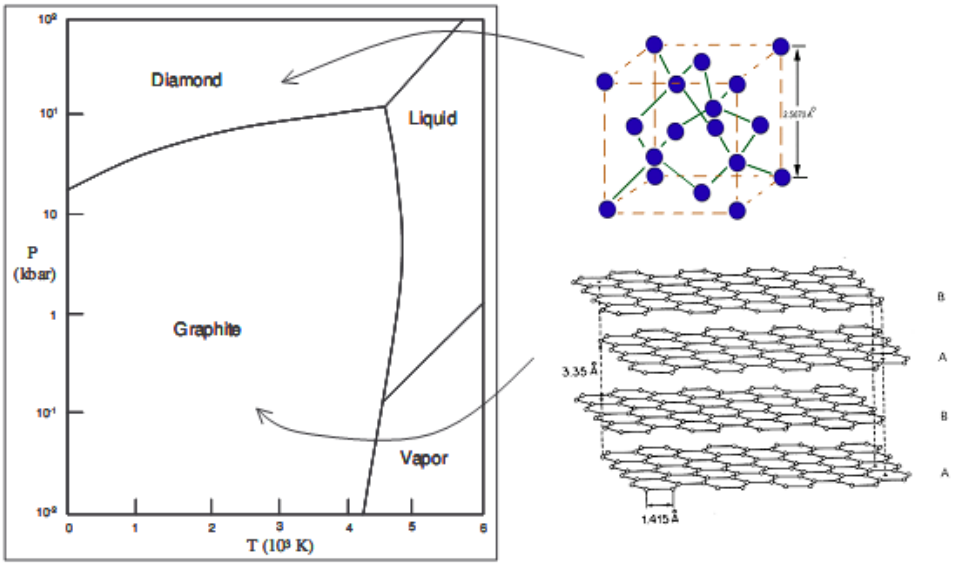


Figure 1.5: Phase diagram for the carbon with the crystal structures of diamond and graphite [19]

The unit cell of graphite can equally be seen on the figure above. Crystalline graphite consists of parallel sheets of carbon atoms, each sheet containing hexagonal arrays of carbon atoms. Each atom is connected to three nearest neighbors, within the sheets, by covalent bonds that separate them by a distance of 1.42 Angstroms.

1.6 Hydrogen Transport and Distribution

Hydrogen can be transported by means of underground pipelines (gaseous hydrogen) and/or supertankers (liquid hydrogen). Presently, hydrogen transportation through pipelines is used either in links between nearby production and utilization sites (up to 10 km) or in more extensive networks (roughly 200 km). Table 1.3 lists the principal existing hydrogen pipelines [20]. For hydrogen pipelines, it is necessary to use steel that is resistant to embrittlement by hydrogen under pressure, particularly for very pure hydrogen (greater than 99.5% purity). Reciprocating compressors used for natural gas can be used for hydrogen without major design modifications. However, special attention must be given to sealing (to avoid hydrogen leaks) and to materials selection for the parts subject to fatigue stress.

As a rule, hydrogen transmission through pipelines requires larger diameter piping and more compression power than natural gas for the same energy throughput. However, due to lower pressure losses in the case of hydrogen, the recompression stations would need to be spaced twice as far apart. In economic terms, most of the studies found that the cost of large-scale transmission of hydrogen is about 1.5-1.8 times that of natural gas transmission.

Table 1.3: Some major hydrogen pipelines [21]

Location	Years of Operation	Diameter (mm)	Length (km)	Pressure (MPa)	Purity
AGEC, Alberta, Canada	Since 1987	273	3.7	3.79	99.9%
Air Liquide, France	Since 1966	various	290	6.48-10	Pure and raw
Air Products, Houston, TX	Since 1969	114-324	100	0.35-5.5	Pure
Air Products, Louisiana	Since 1990	102-305	48	3.45	
Chemische Werke Huls	Since 1938	168-273	215	to 2.5	Raw gas
Cominco, B.C., Canada	Since 1964	5	0.6	>30	62-100%
Gulf Petroleum Canada		168.3	16		93.5%
Hawkeye Chemical, Iowa	Since 1987	152	3.2	2.75	
ICI Bilingham, U.K.			15	30	Pure
Philips Petroleum	Since 1986	203	20.9	12	

Whether produced from fossil or non-fossil sources, the widespread use of hydrogen will require a new and extensive infrastructure to produce, distribute, store and dispense it as a vehicular fuel or for stationary applications, such as electric generation. Depending on the source from which hydrogen is produced and the form in which it is delivered, many alternative infrastructures can be envisioned.

In terms of transportation and distribution, there appears to be general consensus on two broad approaches:

- Small-scale local hydrogen production, based on either electrolysis or gas reformation, thus utilizing existing electricity or gas distribution infrastructure.
- Large-scale dedicated hydrogen production infrastructure, including, pipelines and or road transport.

The first option has a number of attractions from the viewpoint of minimizing distribution costs, although it could make it more difficult to achieve the economies of scale associated with large scale hydrogen production and to capture and store CO_2 when hydrogen is produced out of fossil fuels. It also requires augmentation of both gas and electricity production and distribution infrastructure. This investment could be in addition to that required to integrate renewable energy into the electricity grid system, depending upon the renewable energy sources relative to hydrogen demand centers.

CHAPTER 2

HYDROGEN AS AN ENGINE FUEL

There are a number of unique features associated with hydrogen that make it remarkably well suited in principle, to engine applications. Some of these most notable features are the following:

Hydrogen, over wide temperature and pressure ranges, has very high flame propagation rates within the engine cylinder in comparison to other fuels. These rates remain sufficiently high even for very lean mixtures that are well away from the stoichiometric mixture region. The associated energy release is also so fast that the combustion duration, tends to be short and contributes towards producing high-power output efficiencies and high rates of pressure rise following spark ignition.

The operation on lean mixtures, in combination with the fast combustion energy release rates around top dead center associated with the very rapid burning of hydrogen–air mixtures results in high-output efficiency values. Of course, such lean mixture operation leads simultaneously to a lower power output for any engine size.

One of the most important features of hydrogen engine operation is that it is associated with less undesirable exhaust emissions than for operation on other fuels. As far as the contribution of the hydrogen fuel to emissions, there are no unburned hydrocarbons, carbon monoxide, carbon dioxide, and oxides of sulfur, smoke or particulates. The contribution of the lubricating oil to such emissions in well-maintained engines tends to be rather negligible. Only oxides of nitrogen and water vapor are the main products of combustion emitted. Also, with lean operation the level of NO_x tends to be significantly smaller than those encountered with operation on other fuels.

The fast burning characteristics of hydrogen permit much more satisfactory high-speed engine operation. This would allow an increase in power output with a reduced penalty for lean mixture operation. Also, the extremely low boiling temperature of hydrogen leads to fewer problems encountered with cold weather operation. Varying the spark timing in hydrogen engine operation represents an unusually effective means for improving engine performance and avoidance of the incidence of knock. Also, the heat transfer characteristics of hydrogen combustion in engines are significantly different from those in engines operating on other fuels. The radiative component of heat transfer tends to be small yet the convective component can be higher especially for lean mixture operation.

2.1 Properties of Hydrogen

Hydrogen is the most abundant element in our universe. In addition to being a component of all living things hydrogen and oxygen together make up water, which covers 70 percent of the earth. In its pure form, a hydrogen molecule is composed of two hydrogen atoms (H_2) and is a gas at normal temperatures and pressures. It is the lightest gas with only 7 percent of the density of air.

Hydrogen is an odorless, colorless gas. With molecular weight of 2.016, hydrogen is the lightest element. Its density is about 14 times less than air (0.08376 kg/m^3 at standard temperature and pressure). Hydrogen is liquid at temperatures below 20.3 K (at atmospheric pressure). Some important properties of hydrogen are compiled in Table 2.1.

Table 2.1: Physical properties of hydrogen, methane and gasoline [22]

Property	Hydrogen	Methane	Iso-Octane
Density at 101.325 kPa and 300 K (kg / m^3)	0.082	0.717	5.11
Stoichiometric Composition in air (% by volume)	29.53	9.48	1.65
Stoichiometric Fuel/Air Mass Ratio	0.029	0.058	0.0664
Number of moles after combustion to before	0.85	1.00	1.058
HEATING VALUES H.H.V (MJ/kg) L.H.V (MJ/kg)	 141.7 119.7	 52.68 46.72	 48.29 44.79
H.H.V (MJ/m^3) L.H.V (MJ/m^3)	12.10 10.22	37.71 33.95	233.29 216.38
Combustion energy per kg of stoichiometric mixture (MJ)	3.37	2.56	2.79
Kinematic Viscosity at 300 K (mm^2/s)	110	17.2	1.18
Thermal Conductivity at 300 K (mW/m K)	182.0	34.0	11.2
Diffusion Coefficient Into Air at at 101.325 kPa and 300 K (cm^2/s)	0.61	0.189	0.05

The specific physical characteristics of hydrogen are quite different from those common fuels. Some of those properties make hydrogen potentially less hazardous, while other hydrogen characteristics could theoretically make it more dangerous in certain situations. In Table 2.2 combustion characteristics are shown for certain fuels.

Table 2.2: Combustion properties of hydrogen, methane and gasoline [22]

Property	Hydrogen	Methane	Gasoline
Flammability limits (% by volume)	4 - 75	5.3 - 15.0	1.2 - 6.0
Minimum ignition energy (mJ)	0.02	0.28	0.25
Laminar flame speed at 101.325 kPa and 300 K (m/s)	1.90	0.38	0.37 - 0.43
Autoignition temperature (K)	858	813	~500 - 750

In comparison with the traditional fuels employed regularly now, the hydrogen has many different characteristics. The table 2.3 resumes some selected characteristics of this element.

Table 2.3: Basic properties of hydrogen considering as fuel for combustion engines

Properties	Description
Interval of ignitability	The hydrogen has a wide interval of ignitability in comparison with other fuels; therefore, the hydrogen engines can operate with a higher efficiency and a leaner mixture than the petrol engines. An ignitable mixture is formed as soon as it contains 4% of hydrogen.
Ignition energy	The hydrogen requires lower ignition energy than other fuels. Its disadvantage is the risk of the mixture getting ignited from hot places in the cylinder, and in the equipment serving for the outside formation of the mixture.
Anti-detonation resistance	Up to now, not known to a creditable degree. The results of the tests on the engines and in the research differ.
Burning velocity	The velocity of combustion of the mixture is higher than petrol in the level of orders. It allows for its effective and thorough combustion, even if the burning velocity decreases with leaner mixtures.
Mixture formation	Concerning the formation of the mixture, the gas fuels are more advantageous than the liquid ones because it is easier to mix two substances of the same state. A more perfect use of the air in the combustion and therefore, a better cleanness of the combustion products.
Density	The density of hydrogen is very low, which brings about problems with its storage. Another disadvantage consists in insufficient filling of the cylinder with the fresh mixture.
Calorific value	The calorific value of hydrogen referred to its weight unit is considerably higher than with regular fuels. On the contrary, its volume calorific value is less because of its density.
Extinguishing capacity	It is very low, therefore the mixture can be burnt thoroughly even in remote sections of the combustion room the design of which ought to be adapted in order to avail of this property.
Composition of fuel	It does not contain carbon, positive emissions of the exhaust gases.
Effect upon surrounding materials	Producing the so-called hydrogen brittleness, in particular at higher temperatures and pressures. It is possible chemical reactions with the lubricating oil

2.2 Hydrogen Safety

Like any other fuel or energy carrier hydrogen poses risks if not properly handled or controlled. The risk of hydrogen, therefore, must be considered relative to the common fuels such as gasoline, propane or natural gas.

Since hydrogen has the smallest molecule it has a greater tendency to escape through small openings than other liquid or gaseous fuels. Based on properties of hydrogen such as density, viscosity and diffusion coefficient in air, the propensity of hydrogen to leak through holes or joints of low pressure fuel lines may be only 1.26 (laminar flow) to 2.8 (turbulent flow) times faster than a natural gas leak through the same hole (and not 3.8 times faster as frequently assumed based solely on diffusion coefficients). Since natural gas has over three times the energy density per unit volume the natural gas leak would result in more energy release than a hydrogen leak.

For very large leaks from high pressure storage tanks, the leak rate is limited by sonic velocity. Due to higher sonic velocity (1308 m/s at 100 kPa, 300 K) hydrogen would initially escape much faster than natural gas (sonic velocity of natural gas is 449 m/s). Again, since natural gas has more than three times the energy density than hydrogen, a natural gas leak will always contain more energy. If a leak should occur for whatever reason, hydrogen will disperse much faster than any other fuel, thus reducing the hazard levels. Hydrogen is both more buoyant and more diffusive than either gasoline, propane or natural gas.

Hydrogen/air mixture can burn in relatively wide ratios, between 4% and 75% (by volume) of hydrogen in air. Other fuels have much lower flammability ranges, natural gas 5.3-15%, propane 2.1-10%, and gasoline 1.2-6%. In many actual leak situations the key parameter that determines if a leak would ignite is the lower flammability limit, and hydrogen's lower flammability limit is 4 times higher than that of gasoline, 1.9 times higher than that of propane and slightly lower than that of natural gas.

Hydrogen has a very low ignition energy (0.02 mJ), about one order of magnitude lower than other fuels. The ignition energy is a function of fuel/air ratio, and for hydrogen it reaches minimum at about 20-30% hydrogen content in air.

Hydrogen has a flame velocity 6 times faster than that of natural gas or gasoline. A hydrogen flame would therefore be more likely to progress to a detonation than other fuels. However, the likelihood of a detonation depends in a complex manner on the exact fuel/air ratio, the temperature and particularly the geometry of the confined space. Hydrogen detonation in the open atmosphere is highly unlikely.

The lower detonability fuel/air ratio for hydrogen is 13-18%, which is two times higher than that of natural gas and 12 times higher than that of gasoline. Since the lower flammability limit is 4% an explosion is possible only under the most unusual scenarios, which is, hydrogen would first have to accumulate and reach 13% concentration in a closed space without ignition, and only then an ignition source would have to be triggered. Should an explosion occur, hydrogen has the lowest explosive energy per unit stored energy in the fuel, and a given volume of hydrogen would have 22 times less explosive energy than the same volume filled with gasoline vapor.

Hydrogen flame is nearly invisible, which may be dangerous, because people in the vicinity of a hydrogen flame may not even know there is a fire. This may be remedied by adding some chemicals that will provide the necessary luminosity. The low emissivity of

hydrogen flames means that nearby materials and people will be much less likely to ignite and/or hurt by radiant heat transfer. The fumes and soot from a gasoline fire pose a risk to anyone inhaling the smoke, while hydrogen fires produce only water vapor (unless secondary materials begin to burn).

Liquid hydrogen presents another set of safety issues, such as risk of cold burns, and the increased duration of leaked cryogenic fuel. A large spill of liquid hydrogen has some characteristics of a gasoline *spill*, however it will dissipate much faster. Another potential danger is a violent explosion of a boiling liquid expanding vapor in case of a pressure relief valve failure.

Hydrogen onboard a vehicle may pose a safety hazard. The hazards should be considered in situations when vehicle is inoperable, when vehicle is in normal operation and in collisions. Potential hazards are due to fire, explosion of toxicity. The latter can be ignored since neither hydrogen nor its fumes in case of fire are toxic. Hydrogen as a source of fire or explosion may come from the fuel storage, or from the fuel supply lines.

The largest amount of hydrogen at any given time is present in the tank. Several tank failure modes may be considered in both normal operation and collision, such as: catastrophic rupture, due to manufacturing defect in tank, a defect caused by abusive handling of the tank or stress fracture, puncture by a sharp object, external fire combined with failure of pressure relief device to open; massive leak, due to faulty pressure relief device tripping without cause or chemically induced fault in tank wall; puncture by a sharp object, operation of pressure relief device in a case of fire (which is the purpose of the device); slow leak due to stress cracks in tank liner, faulty pressure relief device, or faulty coupling from tank to the feed line, or impact-induced openings in fuel line connection.

Most of the above discussed failure modes may be either avoided or their occurrence and consequences minimized by: leak prevention through a proper system design, selection of adequate equipment, allowing for tolerance of shocks and vibrations, locating a pressure relief device vent, protecting the high pressure lines, installing a normally closed solenoid valve on each tank feed line; leak detection by either a leak detector or by adding an odorant to the hydrogen fuel; ignition prevention, through automatically disconnecting battery bank, thus eliminating source of electrical sparks which are the cause of 85% gasoline fires after a collision, by designing the fuel supply lines so that they are physically separated from all electrical devices, batteries, motors and wires to the maximum extent possible, and by designing the system for both active and passive ventilation (such as an opening to allow the hydrogen to escape upward).

2.3 Features of Hydrogen for Engine Applications

Theoretically any typical spark-ignited engine, like the gasoline engines used in most cars, can operate on a range of liquid or gaseous fuels, including hydrogen. However, due to differences in the chemical properties of the various fuels, the designs of engines optimized for each are quite different. Because of the wide flammability range of hydrogen, an internal combustion engine (ICE) operating on hydrogen can operate with a much leaner air/fuel mixture than a typical gasoline engine, which improves efficiency. A hydrogen ICE developed by Ford Motor Company can operate with an air excess ratio as high as 2.5, compared to 1 for typical gasoline engines. This results in about a 25 percent improvement in efficiency.

Hydrogen can have a high effective octane number mainly because of its high burning rates and its slow preignition reactivity. Hydrogen has been shown to be an excellent additive in relatively small concentrations, to some common fuels such as methane. Its gaseous state permits excellent cold starting and engine operation. Hydrogen remains in gaseous state until it reaches its condensation point around 20 K. Hydrogen engines are more appropriate for high-speed engine operation mainly due to the associated fast burning rates.

Less spark advance is usually needed, which contributes to better efficiencies and improved power output as the bulk of the heat release by combustion can be completed just after the TDC region. Hydrogen engine operation can be associated with less heat loss than with other fuels. Moderately high compression ratio operation is possible with lean mixtures of hydrogen in air, which permits higher efficiencies and increased power output. Hydrogen engines are very suitable for cogeneration applications since the energy transfer due to condensing some water vapor can add up significantly to the thermal load output and the corresponding energy efficiency.

Hydrogen unlike most other commercial fuels is a pure fuel of well-known properties and characteristics, which permits continued and better optimization of engine performance. The reaction rates of hydrogen are sensitive to the presence of a wide range of catalysts. This feature helps to improve its combustion and the treatment of its exhaust emissions.

The thermodynamic and heat transfer characteristics of hydrogen tend to produce high compression temperatures that contribute to improvements in engine efficiency and lean mixture operation. Hydrogen high burning rates make the hydrogen fueled engine performance less sensitive to changes to the shape of the combustion chamber, level of turbulence and the intake charge swirling effect.

Internal combustion engines can burn hydrogen in a wider range of fuel-air mixtures than with gasoline. Hydrogen with wider flammability limits and higher flame speed makes it more efficient in stop and start driving. Hydrogen can tolerate better the presence of diluents. This would allow a better exploitation of low heating value fuel mixtures. Hydrogen can be employed quite effectively with oxygen-enriched air such as resulting from the electrolysis of water. The gas is highly diffusive and buoyant which make fuel leaks disperse quickly, reducing explosion hazards associated with hydrogen engine operation.

2.4 Limitations associated with hydrogen engine applications

Much of the information reported in the open literature about the performance of engines on hydrogen as a fuel tends to highlight the positive features of hydrogen while de-emphasizing or even ignoring the many limitations associated with such fields of application. There is a need to focus equally well on these and suggest means for overcoming some of their negative aspects. Accordingly, the following is a listing of some features associated with hydrogen as an engine fuel that may be considered as requiring some remedial action:

Hydrogen as a compressed gas at 200 atmospheres and atmospheric temperature has merely around 5% of the energy of gasoline of the same volume. This is a major shortcoming particularly for transport applications. Engines fueled with hydrogen suffer from reduced power output, due mainly to the very low heating value of hydrogen on volume basis and resorting to lean mixture operation. The mass of the intake air is reduced for any engine size because of the relatively high stoichiometric hydrogen to air ratio.

There are serious potential operational problems associated with the uncontrolled preignition and backfiring into the intake manifold of hydrogen engines. Hydrogen engines are prone to produce excessively high cylinder pressure and to the onset of knock. The equivalent octane number of hydrogen is rather low in comparison to common gasoline and methane at the same condition.

The high burning rates of hydrogen produce high pressures and temperatures during combustion in engines when operating near stoichiometric mixtures. This may lead to high exhaust emissions of oxides of nitrogen and produce a high knocking. There are serious limitations to the application of cold exhaust gas recirculation for exhaust emissions control. Hydrogen engines may display some serious limitations to effective turbo charging.

There is always some potential for increased safety problems with hydrogen operation. Hydrogen engine operation may be associated with increased noise and vibrations due mainly to the high rates of pressure rise resulting from fast burning. Great care is needed to avoid materials compatibility problems with hydrogen applications in engines.

In certain applications, such as in very cold climates, the exhaust emission of steam can be an undesirable feature leading to poor visibility and increased icing problems. The sensitivity of hydrogen–air mixtures to catalytic action can be occasionally considered undesirable as it may contribute to reduced safety and poorer control of the combustion process.

Hydrogen requires a very low ignition energy, which leads to uncontrolled preignition problems. There is an increased potential for undesirable corrosion and lubricating oil contamination due to exhaust water vapor condensation. There can be an increased potential for operational durability problems with lubricants.

Heat transfer losses can be high, yet under some conditions they can be quite low. A hydrogen engine operated with lean mixture needs to be some 40–60% larger in size than for naturally aspirated gasoline engine operation for the same power output. This could impose some reduction to engine speed, increased mechanical and motoring losses and reduced tolerance to knocking. Also, some engine design modifications are needed.

2.5 Improving the operational features of SI hydrogen engines

A number of possible changes to the design and operational features of a hydrogen fueled S.I. engine can be suggested to affect the full potential of hydrogen in engine applications. These measures can include the following:

Employ lean mixtures with wide-open throttle. Means are to be provided to apply optimal variable partial throttling at extremely lean mixtures to effect better engine performance. There is a need for uniquely optimized variations in the spark timing throughout so as to improve engine performance while avoiding knock.

The variation in spark timing with hydrogen is more effective in controlling the combustion process than with other fuels. Optimum spark ignition characteristics in terms energy, spark plug gap size and material, plug geometry, electrical insulation etc. need to be employed. Higher engine rotational speeds can be used to increase the power output of an engine operating on hydrogen while maintaining high efficiency and knock free operation.

It is preferable to have timed injection of the hydrogen whether within the manifold or directly into the cylinder, optimized for injection duration, timing and pressure. This is important especially for the avoidance of preignition and backfiring. Provision of some water injection when needed can be also made. Higher compression ratios can be applied satisfactorily to increase the power output and efficiency, mainly because of the relatively fast burning characteristics of the very lean hydrogen–air mixtures.

Carefully controlled cooling of exhaust gas recirculation can be applied for knock avoidance and control. For lean mixture operation with hydrogen suitably heated exhaust gas recirculation can be used. Direct hydrogen gas injection into the cylinder can be applied to produce suitably stratified mixtures for better performance and reduced exhaust emission.

In order to produce a power output comparable with that obtained with other fuels, larger size engines are needed. This will increase somewhat the frictional and motoring losses of the engine. Accordingly, a greater care is needed to reduce these losses so that to retain the high efficiency of hydrogen operation. The volumetric efficiency needs to be maximized so as to enhance the power output.

Uniquely compatible and specially designed turbochargers need to be used for hydrogen engine applications. There is a need to give a greater attention to heat transfer. Also, hotter water jacket temperatures than normally employed for gasoline operations are needed for lean operation. Cooler temperatures need to be employed, however, for high loads with hydrogen and to avoid uncontrolled preignition.

2.6 Engine Modifications

SI engines are relatively adaptable to gaseous fuels like propane, methane, and hydrogen. Slight modifications for the introduction of the fuel in appropriate amount are applied. A fuel supply system that can be tuned according to the engine's need is just good enough to make the engine work. In case of hydrogen there are certain additional issues concerning safety, backfire-safe operation and risk of knocking as well mixture of richness controls throughout the whole operating region. The storage of the fuel is another aspect that affects the range of the vehicle operating on hydrogen. Due to its low energy per volume content, the compressed gas storage cannot compete with liquid gasoline.

Compared to naturally aspirated gasoline engine, hydrogen's low energy per unit volume produces less energy in the cylinder. An engine running on hydrogen produces less power than with gasoline. Supercharging may help remedy this by compressing the incoming fuel/air mixture before it enters the cylinder. This increases the amount of energy per volume of fuel. Additional weight and complexity is added to the engine by such modifications. But the power gain and backfire resisting property (by cooling the cylinder with more air) compensates for the mentioned drawbacks. However, the risks of backfire will occur for external mixture formation engine.

2.7 Mixture formation and engine operation

The extreme physical properties of hydrogen at ambient and cryogenic conditions are beneficial influence on combustion as well as on mixture formation. In contrast to conventional fuels, the hydrogen fraction in a stoichiometric mixture at ambient temperature is about 30% of the mixture volume. The volumetric heat value of the hydrogen-air mixture (2890 J/dm^3 at 100 kPa, 300 K) results in a corresponding power loss at the engine compared to conventional fuel (3900 J/dm^3).

The wide flammability range of H_2-air mixtures enables very lean operation with substantially reduced NO_x emissions much more easily than with conventional fuels. Also, hydrogen offers a considerable reduction of air throttle and cylinder charge intake flow losses. In this point hydrogen differs considerably from other gaseous fuels such as natural gas or propane.

2.7.1 Mixture formation with hydrogen at ambient conditions

Substantial reduction of NO_x emissions is demonstrated with lean mixture concepts without using catalysts at the exhaust system. To achieve satisfactory engine operation several additional measures are necessary to prevent uncontrolled pre-ignition and backfiring into the intake manifold. Supercharging is an additional measure to compensate for the loss of power output, which is related to the lean mixture concepts.

Two basic approaches have been taken to obtain a combustible hydrogen/air mixture in the cylinder of an ICE: external and internal mixture formation, each of which in turn is further subdivided into separate lines.

2.7.2 External mixture formation

In this approach the mixture of hydrogen and air is formed outside the cylinder, including usually the early part of the inlet stroke. It is thus characterized as being at essentially ambient pressure, and at a temperature from near-ambient down depending on hydrogen storage temperature.

At its simplest, the hydrogen can come from a single device that meters the quantity for each cylinder in turn. This would be analogous to the single carburetor of simple gasoline engines, but has the great disadvantage for hydrogen of making the whole inlet manifold subject to backfire. Somewhat more complicated is the timed injection where each inlet port is supplied with low-pressure hydrogen, limiting the backfire-prone mixture to that in the immediate vicinity of each cylinder.

At low engine speed and load, hydrogen combustion with external mixture formation proceeds smoothly over a wide range of lean mixtures. Thermal efficiencies are high, and the exhaust contains only trace quantities of NO_x (the low temperatures of lean mixtures block NO_x formation), as well as inevitable traces of CO and CO_2 typical of lubricating oil combustion. Unfortunately, this excellent result starts deteriorating toward mid-powers and speeds with the advent of rough combustion caused by pre-ignition and backfire. The NO_x levels can increase rapidly and power levels typical of gasoline engines cannot be achieved, not only because of hydrogen's low density, but also because of deteriorating combustion.

The phenomena at work in irregular combustion during the inlet stroke have no doubt been investigated by most researchers, but the most complete reporting has been made by Musashi Institute of Technology. Koyanagi [23] describe the definitive experiments on a single-cylinder engine supplied with hydrogen from a relatively large reservoir with spark plug ignition at 231 BTDC and 10:1 or 12:1 compression ratio. Temperatures were measured by thermocouples near the surface of the spark plug, object lenses followed the luminescence of the flame, recorded either by photomultiplier or by high-speed video camera, and of course crank angle and internal pressures were recorded. They found that:

- Backfiring occurred more easily and frequently with leaner mixtures and at the lower compression ratio, i.e., at lower temperatures.

- The spark plug can be eliminated from consideration as the source of pre-ignition and backfire.
- Special pistons with enlarged radial clearance at top land clearly showed that the exhaust gases trapped in this clearance volume were the source of pre-ignition and backfire.

Because little can be done to eliminate such residual pockets of hot exhaust gas, the Musashi researchers seem to have abandoned external mixture formation, because most of their remaining reports deal only with internal mixture formation. Others prefer to continue with the external mixture formation, and ascribe the backfire to other causes such as spark plugs and hot exhaust valves, but they try to get around the problem by two lines of approach:

- A mechanical/hydraulic one, in which cool air first enters the cylinder, ambient-temperature gaseous hydrogen (GH_2) is injected at low pressure, further air flow purges the inlet port of hydrogen, and the inlet valve closes; the low temperatures retard pre-ignition and even if it occurred, the flame does not backfire into the inlet port.
- A cryogenic one, in which low-temperature gaseous or liquid hydrogen (LH_2) is injected into the inlet port retarding any pre-ignition at least until the inlet valve is closed and backfire becomes impossible.

2.7.3 Internal Mixture Formation

Internal mixture formation refers to H_2 injection with all valves closed, generally as the piston approaches TDC and before ignition is sparked. It requires pressures as high as 100 bar, especially as the advantage of high compression ratios (higher power and efficiencies) can be exploited. Therein lies the challenge because only LH_2 can be considered mixing must be accomplished in very few milliseconds; and cryogenic pumps and injectors when cavitation is always incipient, and the fluid has no lubricating potential, simply do not exist except in experimental versions.

With internal fuel mixing air and fuel are mixed inside the combustion chamber. This is generally done as follows: air is taken in which also cools any hot spots in the cylinder, air intake valve is closed, fuel is injected, fuel inlet valve is closed, the mixture is ignited. When hydrogen is inducted into the cylinder under pressure no air is displaced in the combustion chamber. This prevents the power loss from externally mixed fuel-air systems. Theoretically, 20% more power is possible with directly injected hydrogen fuel than with the same engine using externally mixed gasoline. Hydrogen is injected immediately after the intake valve closes during compression stroke and before the combustion chamber pressure reaches maximum.

There are two types of internal mixture formation: early injection and late injection. With early injection, fuel is introduced at the start of the compression stroke and continues until 90 °BTDC. With late injection, fuel is introduced at 5 °BTDC. High pressure is needed to get enough fuel into the chamber in a short time. With liquid hydrogen fuel, the fuel pump can supply some of this pressure. Fuel expansion from evaporating liquid hydrogen supplies the rest of the 100 bar pressure needed. Fuel injection in general and late injection in particular, makes fuel-air mixing difficult because of the short time involved. Uneven mixtures cause: increased nitrous oxide formation, erratic ignition, ignition delay, incomplete combustion, delayed combustion. These problems can be overcome by increasing the turbulence in the combustion chamber.

2.8 Hydrogen fueled engine applications

The use of hydrogen as an engine fuel has been attempted on very limited basis with varying degrees of success by numerous investigators over many decades [24], and much information about their findings is available in the open literature. However, these reported performance data do not necessarily display consistent agreement between various investigators. There is also a tendency to focus on results obtained in specific engines and over narrowly changed operating conditions. Moreover, the increasingly greater emphasis being placed on the nature of emissions and efficiency considerations often renders much of the very early work fragmentary and mainly of historical value.

Obviously, there is a need to be aware of what has been achieved in this field while focusing both on the attractive features as well as the potential limitations and associated drawbacks that need to be overcome for hydrogen to become a widely accepted and used fuel for engine applications. Also, there is a need to indicate practical steps for operating and design measures to be developed and incorporated for hydrogen to achieve its full potential as an attractive and superior engine fuel.

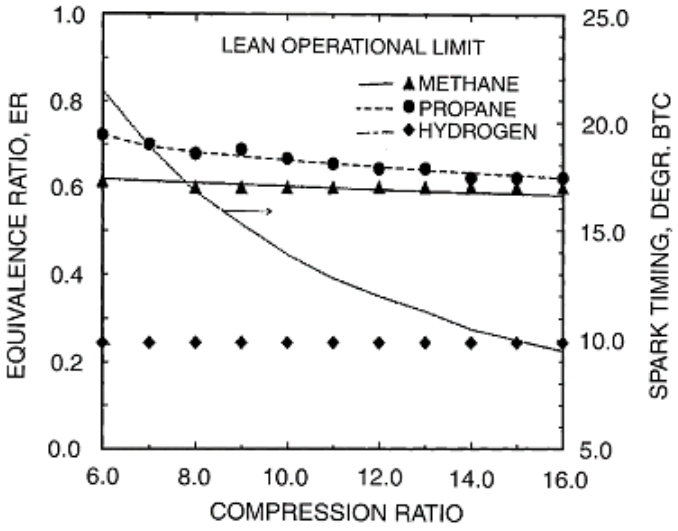


Figure 2.1: Variations of the lean operational limits(ER) or air excess ratio (λ), where is λ=1/ER with changes in compression ratio for different gaseous fuels at 900 rpm. [25]

There are a number of unique features associated with hydrogen that make it remarkably well suited in principle, to engine applications. Some of these most notable features are the following [25]:

(i) Hydrogen, over wide temperature and pressure ranges, has very high flame propagation rates within the engine cylinder in comparison to other fuels. These rates remain sufficiently high even for very lean mixtures that are well away from the stoichiometric mixture region. The associated energy release is also so fast that the combustion duration and tends to be short and contributes towards producing high-power output efficiencies and high rates of pressure rise following spark ignition [26].

(ii) The lean operational limit mixture in a spark ignition engine when fuelled with hydrogen is very much lower than those for other common fuels, as shown typically in

Fig.2.1 for a range of compression ratios. This permits stable lean mixture operation and control in hydrogen fueled engines [27].

(iii) The operation on lean mixtures, in combination with the fast combustion energy release rates around top dead center associated with the very rapid burning of hydrogen-air mixtures results in high-output efficiency values [28]. Of course, such lean mixture operation leads simultaneously to a lower power output for any engine size.

(iv) One of the most important features of hydrogen engine operation is that it is associated with less undesirable exhaust emissions than for operation on other fuels. As far as the contribution of the hydrogen fuel to emissions, there are no unburnt hydrocarbons, carbon monoxide, carbon dioxide, and oxides of sulfur, smoke or particulates [29]. The contribution of the lubricating oil to such emissions in well-maintained engines tends to be rather negligible. Only oxides of nitrogen and water vapor are the main products of combustion emitted. Also, with lean operation the level of NO_x tends to be significantly smaller than those encountered with operation on other fuels [30].

(v) The fast burning characteristics of hydrogen permit much more satisfactory high-speed engine operation [31]. This would allow an increase in power output with a reduced penalty for lean mixture operation. Also, the extremely low boiling temperature of hydrogen leads to fewer problems encountered with cold weather operation.

2.8.1 Some other positive features of hydrogen for engine applications

In addition to the previous unique features associated almost exclusively with hydrogen, a number of others can be cited in support of hydrogen applications in engines. The following is a listing of some of the main of these features:

• Less cyclic variations are encountered with hydrogen than with other fuels, even for very lean mixture operation. This leads to a reduction in emissions, improved efficiency, and quieter and smoother operation.
• Hydrogen has been shown to be an excellent additive in relatively small concentrations, to some common fuels such as methane [32].

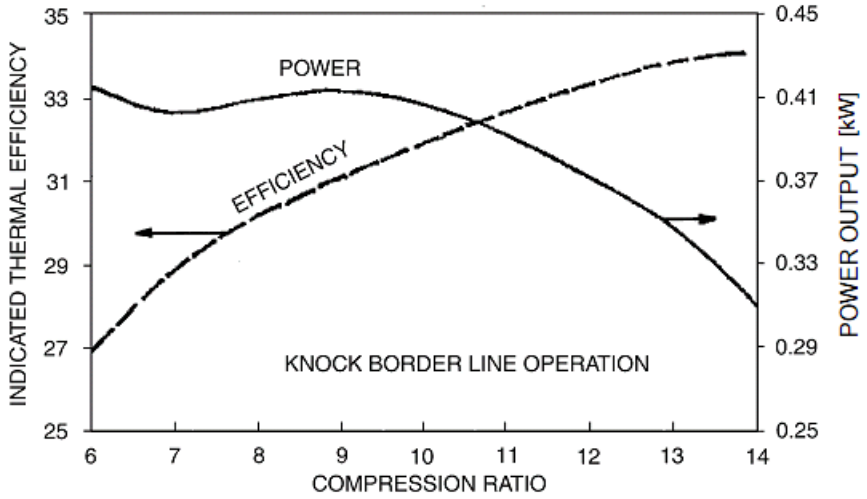


Figure 2.2: Typical variations in indicated power output and efficiency (CFR engine) with changes in compression ratio when using optimum spark timing for borderline knock [33].

• Hydrogen engines are more amenable to high-speed engine operation mainly due to the associated fast burning rates.
• Less spark advance is usually needed, which contributes to better efficiencies and improved power output as the bulk of the heat release by combustion can be completed just after the TDC region.
• Moderately high compression ratio operation is possible with lean mixtures of hydrogen in air, which permits higher efficiencies and increased power output, as shown in figure 2.2
• Hydrogen engines are very suitable for cogeneration applications since the energy transfer due to condensing some water vapor can add up significantly to the thermal load output and the corresponding energy efficiency.
• The thermodynamic and heat transfer characteristics of hydrogen tend to produce high compression temperatures that contribute to improvements in engine efficiency and lean mixture operation.
• Hydrogen high burning rates make the hydrogen fueled engine performance less sensitive to changes to the shape of the combustion chamber, level of turbulence and the intake charge swirling effect.
• Hydrogen can tolerate better the presence of diluents. This would allow a better exploitation of low heating value fuel mixtures.

2.8.2 Some limitations associated with hydrogen engine applications

Much of the information reported in the open literature about the performance of engines on hydrogen as a fuel tends to highlight the positive features of hydrogen while de-emphasizing or even ignoring the many limitations associated with such fields of application. Accordingly, the following is a listing of some features associated with hydrogen as fuel that may be considered as requiring some remedial action:

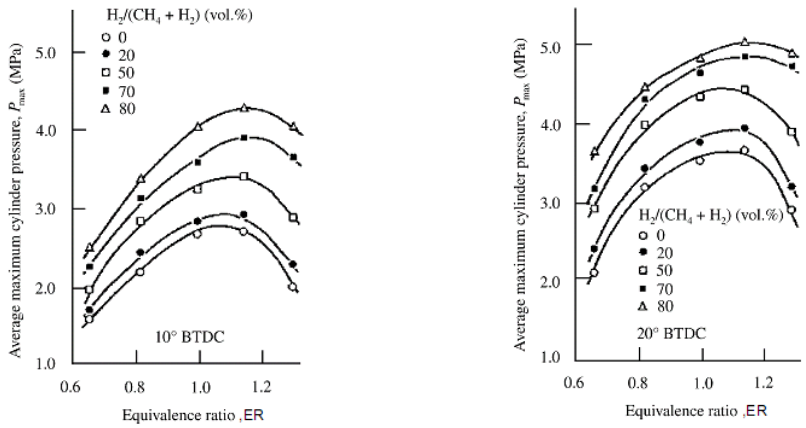


Figure 2.3: Typical variations in the maximum cylinder pressure with changes in equivalence ratio (ER) or air excess ratio (λ), where is λ = 1/ER, when operating on a range of fuel mixtures of hydrogen and methane for two spark timings [34].

• Hydrogen as a compressed gas at 200 atmospheres and atmospheric temperature has merely around 5% of the energy of gasoline of the same volume. This is a major shortcoming particularly for transport applications.

• The naturally aspirated engine engines fueled with hydrogen suffer from reduced power output, due mainly to the very low heating value of hydrogen on volume basis and resorting to lean mixture operation.

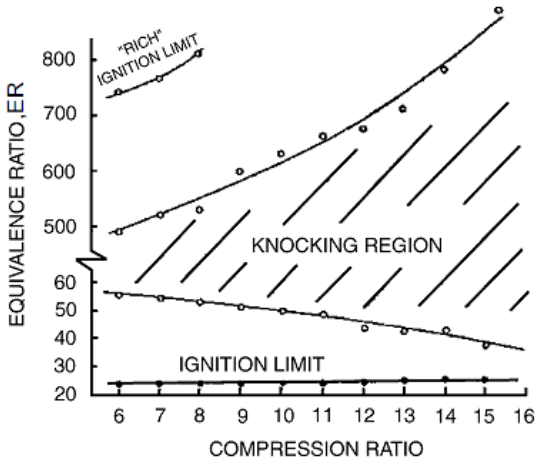


Figure 2.4: Variations of operational limits for ignition and knock with ratio(ER) or air excess ratio (λ), where is λ = 100/ER, changes for hydrogen operation at ambient intake conditions [35].

2.8.3 Some measures for improving the operational features of SI hydrogen engines

A number of possible changes to the design and operational features of a hydrogen fueled S.I. engine can be suggested to effects the full potential of hydrogen in engine applications. These measures can include the following:

(i) Employ lean mixtures with wide-open throttle. Means are to be provided to apply optimal variable partial throttling at extremely lean mixtures to effect better engine performance.

(ii) There is a need with hydrogen as a fuel for uniquely optimized variations in the spark timing throughout so as to improve engine performance while avoiding knock. The variation in spark timing with hydrogen is more effective in controlling the combustion process than with other fuels.

(iii) Higher engine rotational speeds can be used to increase the power output of an engine operating on hydrogen while maintaining high efficiency and knock free operation.

(iv) It is preferable to have timed injection of the hydrogen whether within the manifold or directly into the cylinder, optimized for injection duration, timing and pressure. This is important especially for the avoidance of preignition and backfiring. Provision of some water injection when needed can be also made [36].

(v) Higher compression ratios can be applied satisfactorily to increase the power output and efficiency, mainly because of the relatively fast burning characteristics of the very lean hydrogen-air mixtures.

(vi) Direct hydrogen gas injection into the cylinder can be applied to produce suitably stratified mixtures for better performance and reduced exhaust emission.

(vii) The volumetric efficiency needs to be maximized so as to enhance the power output.

When these measures are implemented in the design and operation of hydrogen fuelled spark ignition engines, then most of the apparent limitations associated with hydrogen as an engine fuel will be substantially minimized. Moreover, hydrogen engine operation can be shown to possess operational characteristics that are superior to those associated with other more conventional fuels.

2.9 Experience with the piston hydrogen engine at Department of Vehicles and Engines on Technical University of Liberec

The hydrogen piston engines can be based on the concepts of both the external and internal formation of the mixture, and they can operate both a naturally aspirated engine and a supercharged engine. The external formation of the mixture system (mixer, blower or injector in the suction manifold of the engine) is simpler in the requirements upon the design. However, in the non-supercharged engine the specific output of the hydrogen engine is relatively low (the large specific volume of hydrogen reduces the weight filling of the cylinder with a fresh mixture); this problem can be eliminated by a supercharged engine only.

The external formation of the mixture is accompanied with the risk of a preignition of the mixture prepared in the suction manifold of the engine (due to a very low of activating energy necessary to ignition of hydrogen & air mixtures). The internal formation of the mixture suppresses the risk of a preignition and backfires into the suction manifold. However, the blowing or the injection of hydrogen directly into the combustion chamber reduces the time for the preparation of the mixture, and weaken the mixing of hydrogen with the air (with negative effects upon the chemical effectiveness of the combustion). The solution can consist in injection of hydrogen direct to the cylinder at the end of the suction stroke, and an intensive turbulence (squish swirl) in the cylinder (combustion chamber).

The experimental research program on hydrogen SI engine has been conducted at laboratory of Department vehicle and engines on Technical University of Liberec for 15 years. The majority of the experiments on the testing single-cylinder engine in the laboratory of the Technical University of Liberec has been realized with internal formation of the mixture (by means of a injector specially designed for the testing engine, with the electronically controlled valve – the hydrogen pressure of 1 MPa is input to injector valve).

Figure 2.5 indicates a layout of experimental single-cylinder engine with ECU accessories for mixture forming using direct injection of hydrogen to cylinder engine. The research program on experimental single-cylinder engine concerned the metering on natural aspirated engine and supercharged engine (supercharged using external sources of compressed air). With regard to relatively high coefficient of air excess in hydrogen-air mixtures the required charging pressure of air are also relative high (for requirements to achieve the power parameters of hydrogen engine comparable to parameters of existing SI engine). The different values on charging pressure are required between the way of mixtures creation with direct injection of hydrogen during sucking stroke and the other approach was direct hydrogen injection during compression stroke (after inlet valve closed or after TDC).

Results of performed experiments demonstrate that the hydrogen engine is able to reliably operate at wide range of mixture richness. With respect to very low knocking resistance of hydrogen, the engine was set on very poor mixture combustion (values of air excess coefficient (λ), range from 1.8 to 2.65). The former researches on experimental single-cylinder engine also are showed on different injection time between the combustion course of hydrogen-air for injection of hydrogen during suction stroke and compression stroke.

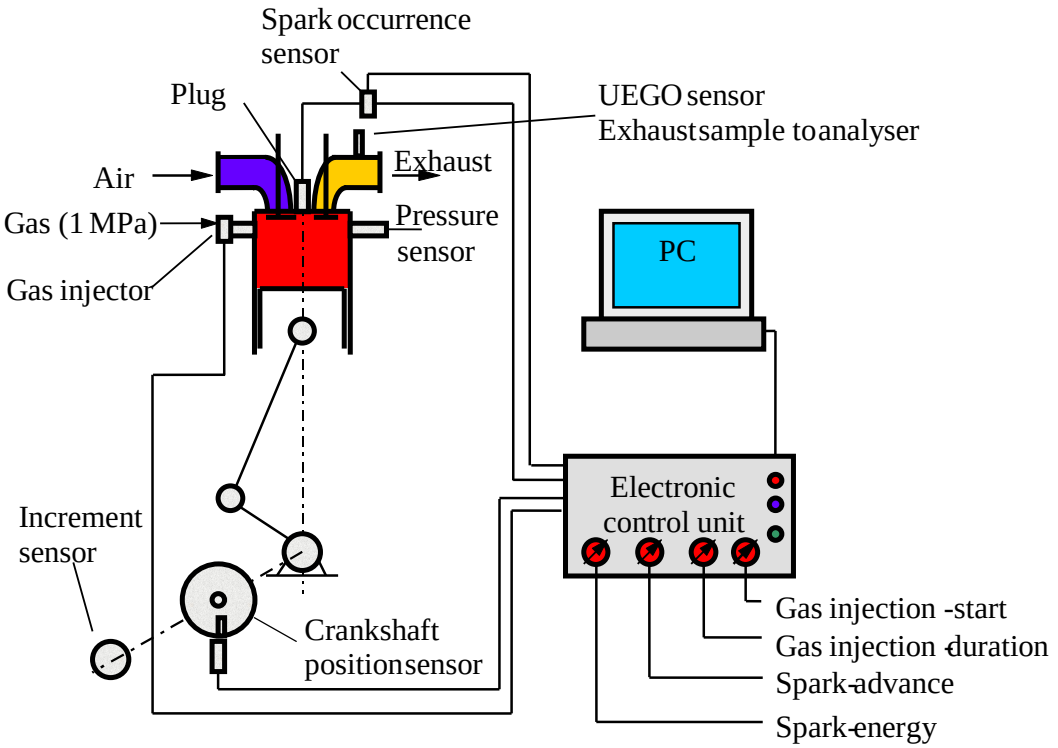


Figure 2.5: Experimental single cylinder engine on hydrogen fuel be created by conversion of original single-cylinder engine OKC octane (CFR engine). Except changes of fuel system and whole accessories the single-cylinder engine was modified for running at speed n=1500 rpm. Major part experimental program has been performed at compression ratio engine ε=10. Direct injection of hydrogen to the engine cylinder has been possible to control during suction and compression stroke [37].

The direct injection of hydrogen to the cylinder during compression stroke (after closed inlet valve) evidently leads to certain inhomogeneity of mixtures, which at directions of fuel spray to spark plug leads to local mixture enrichment and induces the combustion with knocking. The combustion course of p-α diagram by from measurements on hydrogenous experimental single-cylinder engine are indicated on figure 2.6 to 2.8 (diagrams show the cycles with the highest, the mean and the lowest values of p_{max} – selected from the set of 150 cycles).

For the increasing of engine power parameters, the injection pressure of 1 MPa has been low. The further research, therefore, has been prepared the experimental 3-cylinder automotive SI engine with internal mixture formation using high pressure injection of gaseous fuels (natural gas or hydrogen, potential mixtures of these gases). Description of this testing bench and selected experience from experimental research on this hydrogen engine will be described at following parts of paper.

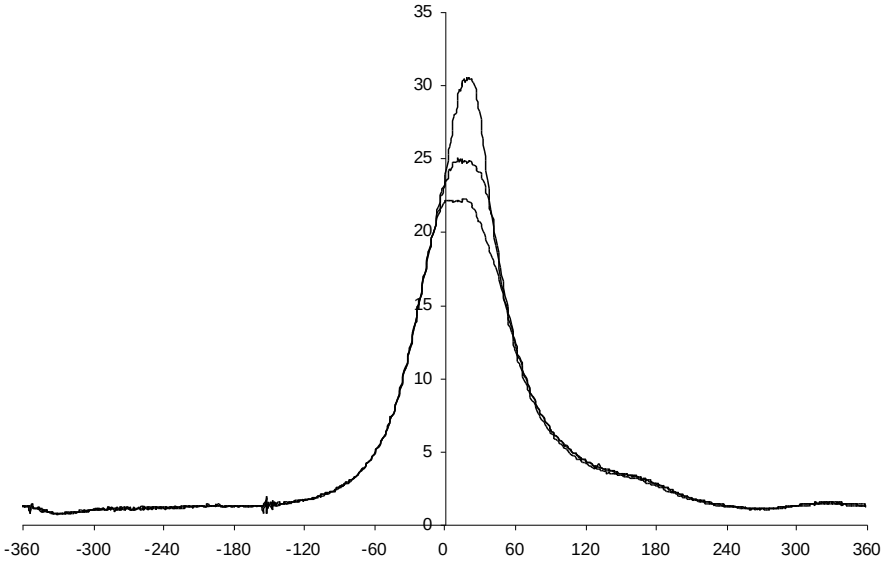


Figure 2.6**:** Pressure courses in the cylinder of the piston combustion engine at the operation with a very lean hydrogen & air mixture: operating range of 1500 1/min, p_i=0.535 MPa, $VARp_i$=5.01%, $VARp_{max}$=7.04%. Supercharging with air Δp=39 kPa, injection of the hydrogen into the cylinder during the suction stroke, air excess λ=2.65 and advance of ignition 5°BTDC. The measured concentration of NO_x=28 ppm [37].

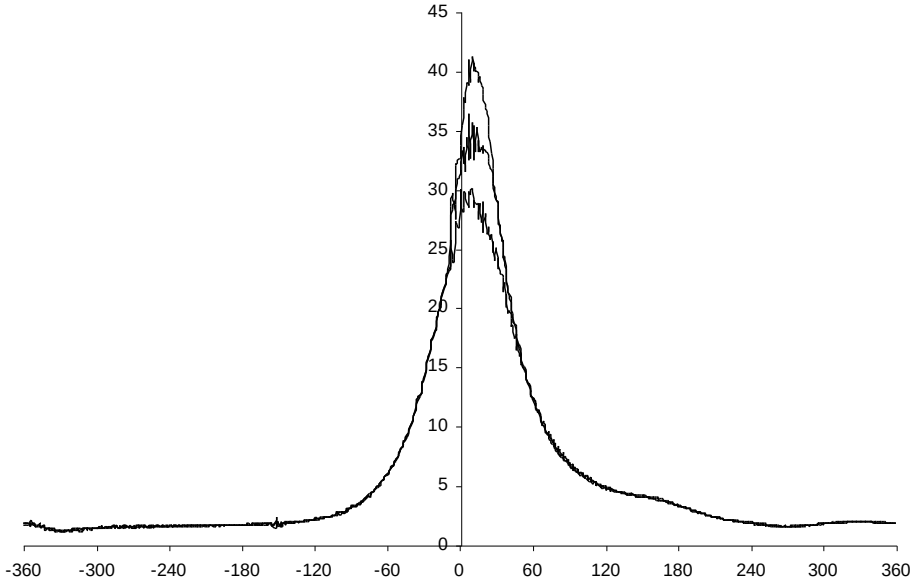


Figure 2.7: Pressure courses in the cylinder of the piston combustion engine at the operation with a very lean hydrogen & air mixture: operating range of 1500 1/min, p_i=0.536 MPa, $VARp_i$=3.42%, $VARp_{max}$=6.35%. Supercharging with air Δp=39 kPa, injection of the hydrogen into the cylinder during the compression stroke, air excess λ=2.65 and advance of ignition 5°BTDC. The measured concentration of NO_x=212 ppm [37].

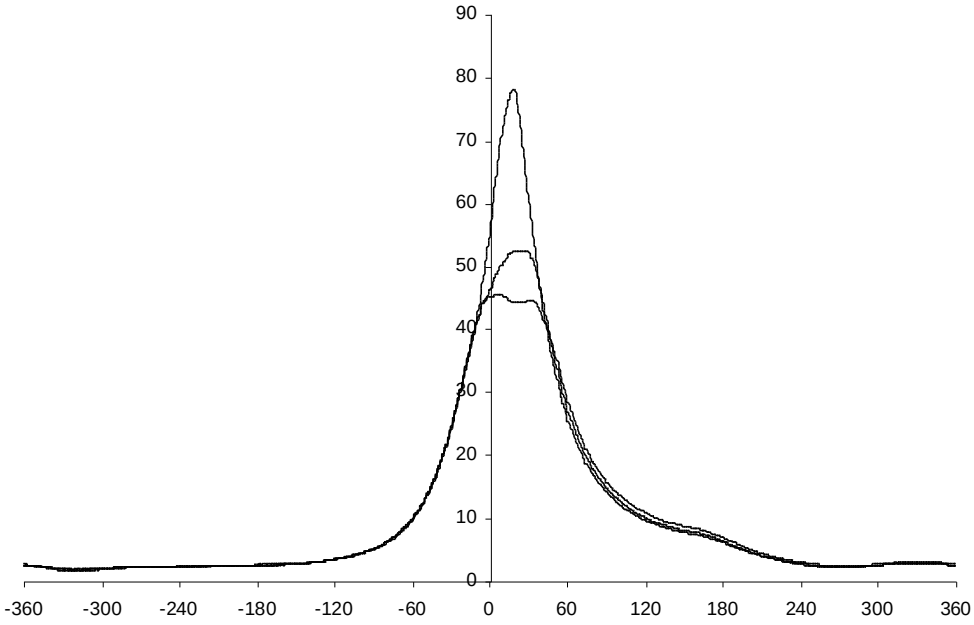


Figure 2.8: Pressure courses in the cylinder of the piston combustion engine at the operation with a very lean hydrogen & air mixture: operating range of 1500 1/min, p_i=1.237 MPa, $VARp_i$=6.13%, $VARp_{max}$=13.3%. Supercharging s Δp=180 kPa, injection of the hydrogen into the cylinder during the suction stroke, air excess λ=2.33 and advance of ignition 5°BTDC. The measured concentration of NO_x=28 ppm [37].

2.10 Results of NO_x production by GT-Power simulation

At sequence of experimental research work with the hydrogen engine at Department laboratory at Technical university of Liberec the computational solution of NO forming were performed at Czech Technical University at Prague as show in figure 2.9 and 2.10.

Proper simulation of the thermal NO_x formation is important in the case of the hydrogen-fueled engine since a formation of prompt NO_x can be neglected because of the lack of HC radicals [38]. The main problem connected to the NO_x formation modeling arises from the characteristic time of the slow NO_x formation reactions. The slow kinetics requires solving of the stiff and computationally demanding chemistry much longer time than it is necessary to solve the combustion to be able to predict the NO_x concentration in the exhaust.

The influence of spark timing, respectively start-of-combustion, is shown in figure. 2.6 and 2.7. All simulations have been performed at constant air excess of 2. Start of combustion angle has a very strong impact on NO_x formation due to the decreasing in-cylinder temperatures if retarding spark advance timing.

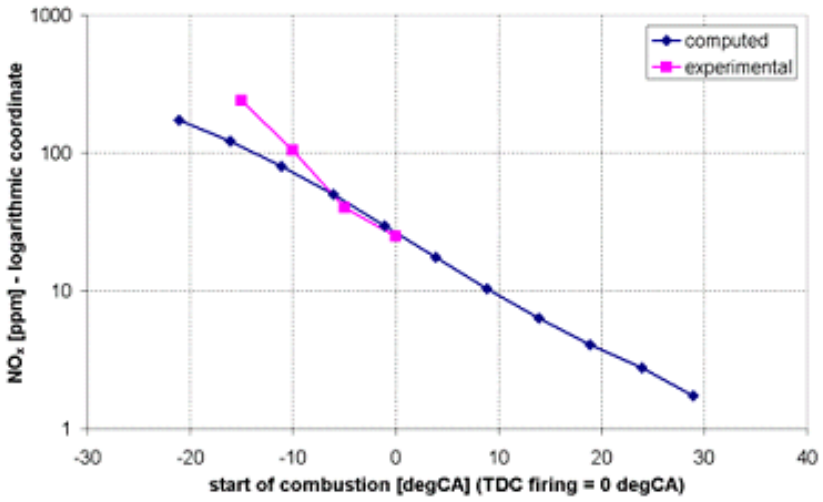


Figure 2.9: Influence of start of combustion on NO_x production with air excess of 2, compression ratio of 10, speed of 910 rpm and homogeneous charge combustion. Comparison of computed and measured data is indicated. [39]

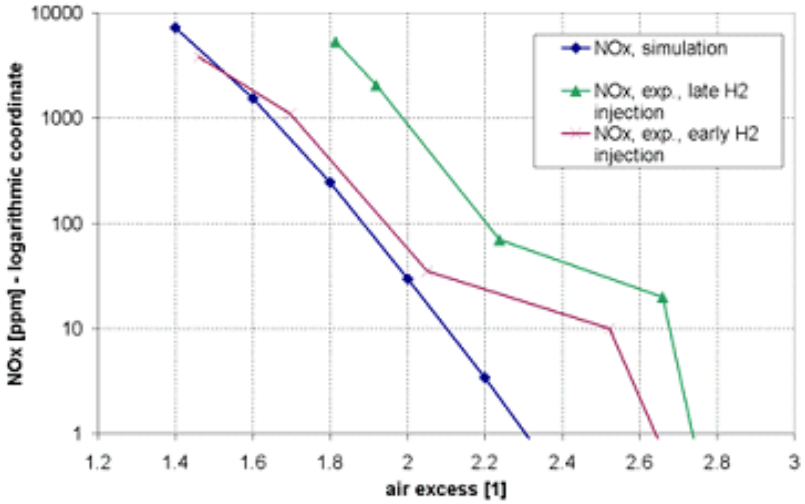


Figure 2.10: Influence of air excess on NO_x production. Spark advance of 5 °BTDC, compression ratio of 10, 910 rpm. homogeneous charge combustion (*early injection timing*). Experimental results of stratified mixture combustion are also plotted (*late injection timing*). [39]

The influence of air excess at constant spark timing of 5 °BTDC is shown in figure. 2.10. In figure 2.10 the comparison of computed and measured NO_x concentration in exhaust gases is presented. Two cases have been examined experimentally – premixed mixture combustion and stratified mixture one. Results show very strong dependence of NO_x formation on air excess.

2.11 An hydrogen engine application

MAN Company developed the naturally aspirated hydrogen engine with external mixture formation and turbocharger engine with internal mixture formation for bus. The result indicated the improvement both NO_x formation and their characteristics performance in figure 2.11 to 2.13.

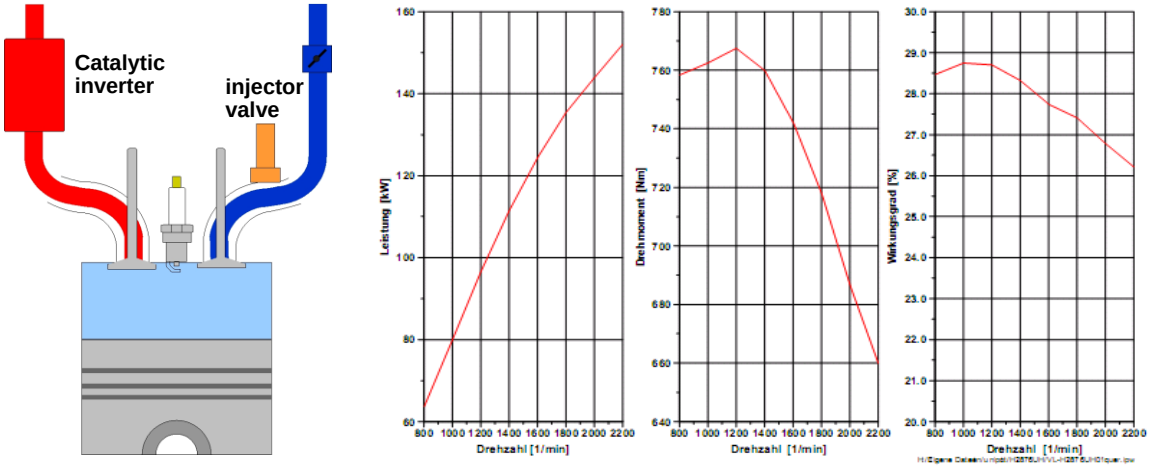


Figure 2.11: Characteristics performance of naturally aspirated hydrogen engine with external mixture formation ($\varepsilon = 8$ and $\lambda = 1$). The graphs indicate low of output power and efficiency [40].

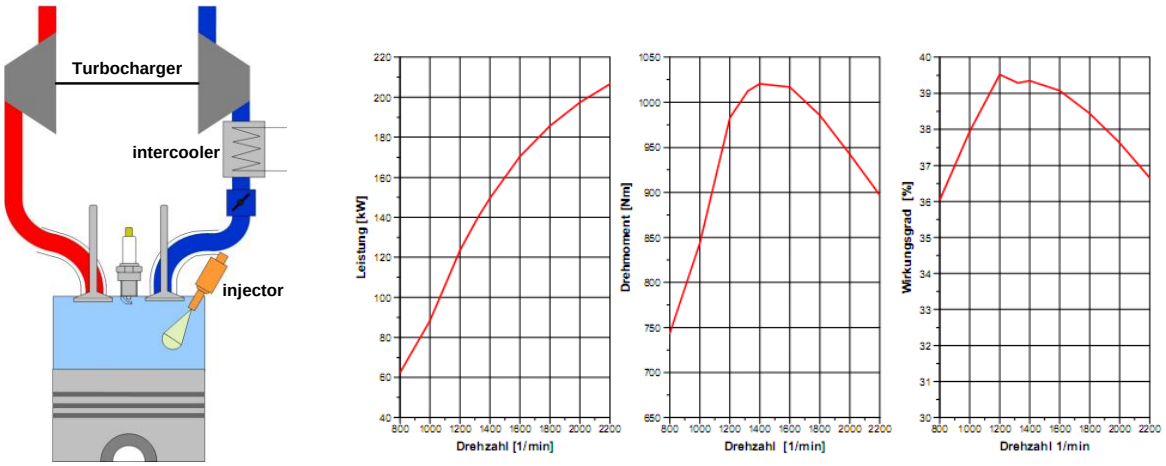


Figure 2.12: Characteristics performance of direct injection hydrogen SI engine with turbocharger and intercooler ($p_{inj} < 10$ bar, $\varepsilon = 12$ and $\lambda > 2$). The graphs indicate higher specific power output and improved efficiency compared with conventional hydrogen engine with external mixture formation [40].

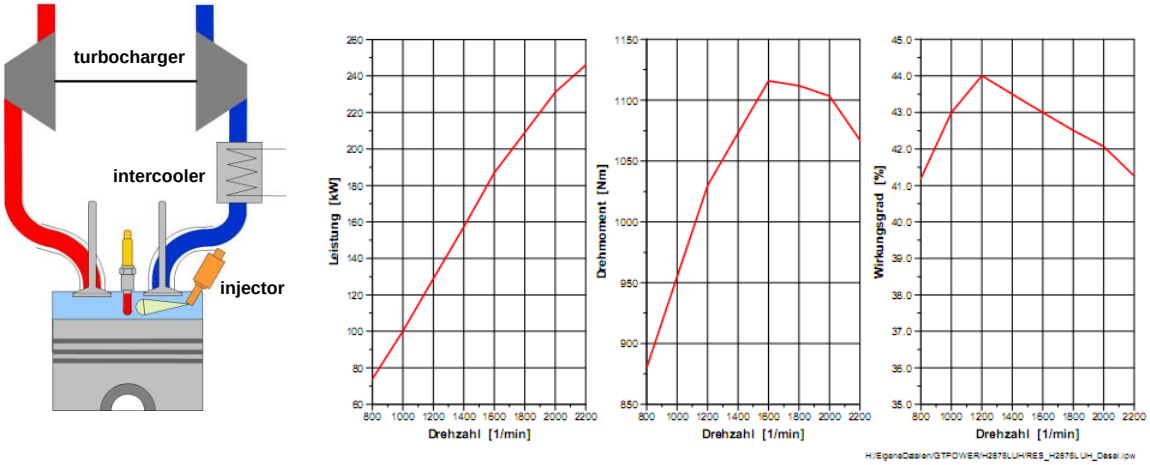


Figure 2.13: Characteristics performance of internal mixture formation hydrogen SI engine with turbocharger, inter cooler and glow plug (p_{inj} ~ 200 bar, ε = 18 and λ is variable). The specific power output and improved efficiency are improved [40].

This chapter has been focused on the fundamental properties of hydrogen compared to the usual hydrocarbons, which are often the same as those of interest to safety. It also describes the two delivery system direct and port injection with hydrogen. Advantages and disadvantages of using hydrogen as alternative fueled were investigated. In addition, TUL laboratory conducted the experimentation on single cylinder engine using hydrogen to study injection time effect on NO_x level in emission. Moreover, MAN company developed a direct injection system for hydrogen fueled engine compared to external mixture formation system and the result showed an improved performance of engine.

CHAPTER 3

THE GOALS OF THESIS

3.1 Motivation

Gasoline and diesel engines are large contributors to urban air pollution. Carbon dioxide and unburned hydrocarbon emissions from engines contribute to global warming. Nitrogen oxides and hydrocarbon react in the atmosphere to form photochemical smog. Particulate matter from diesel engines increases rates of asthma and respiratory problems. In an attempt to reduce the air pollution from engine, researchers have studied alternative sources of power for transportation such as hybrid gasoline-electric cars and fuel-cell cars. These alternatives have shown potential to be clean sources of power for transportation but involve considerable extra manufacturing costs and untested technologies. Another alternative technology is the hydrogen as a spark ignition engine, which uses largely conventional internal-combustion engine technology.

The research shows the wide range of the problems, joint with the research of conditions and the suitable solution for the implementation of hydrogen like engine fuel for the vehicles piston internal combustion engine. This dissertation work is focused to one part of significant area of hydrogen technology, on creation of mixtures and their combustion in piston gas-engine.

Regarding to the safeness work with hydrogen at the experimental research on the test engine has been the whole program of dissertation work restricted on the study problems of internal creation of hydrogen-air mixtures using the high pressure direct injection (gas blow) of the gaseous hydrogen to the engine cylinder and on the combustion of mixtures created too.

3.2 Objectives of Thesis

The dissertation work also refers to former experimental program with hydrogen single cylinder engine at Department laboratory, Technical University of Liberec. That is why that the thesis occupies to creation and combustion only poor mixture. Reason for this delimitation of the experimental program was partly the very intensive engine knocking at combustion of the mixture with the low air excess and high risk of the test engine damage, in part to ascertain the possibilities for achievement of very low NO_x concentration in exhaust gas without using the catalytic converter. The aims of this dissertation work which relate and continue the previous experimental research at department laboratory, Technical University of Liberec were determined by this way:

1. This project is set up for extension study on single cylinder engine using hydrogen which performed at the Engines Laboratory of Technical University of Liberec for 15 years ago. At present, this study examines the effect of injection timing, ignition timing, injection pressure and air to fuel ratio on performance characteristics and NO_x and unburned hydrogen content in emission for 3-cylinder conventional spark ignition engine with

modified direct injection of hydrogen fuel system at 3000 rpm. Comparison is made between CNG and hydrogen operation.

2. Experimental research on testing hydrogen engine. Evaluation of the combustion process parameters, power cycle parameters and emission engine characteristics depend on operating mode and engine adjustment.

3. Determination of parameters for cylinder charging of fresh air to achievement of required power quality of testing piston hydrogen engine with internal creation of poor hydrogen-air mixture by simplified computational program calculation which was developed by department of motors and vehicles, Technical University of Liberec. In addition, computational estimation of NO_x concentration in exhaust gas of hydrogen engine for choice of the setting and operating mode of engine using the program developed by department of motors and vehicles, Technical University of Liberec. Finally, analysis of results and piece of knowledge from performed works and conclusions.

CHAPTER 4

EXPERIMENTS ON SI ENGINE WITH HYDROGEN DIRECT INJECTION

The experimental research program on hydrogen SI engine has been conducted at laboratory of Department vehicle and engine on Faculty of Engineering Technical University of Liberec for 15 years. The majority of the experiments on the testing single-cylinder engine in the laboratory of the Technical University of Liberec has been realized with internal formation of the mixture (by means of a injector specially designed for the testing engine, with the electronically controlled valve – the hydrogen pressure of 1 MPa is input to injector valve).

4.1 Experimental hydrogen direct injection engine

Fuel mixture formation inside the cylinder has become more prevalent in spark ignition engines in recent years. This concept can be beneficially utilized in hydrogen internal combustion engines where direct injection into an engine cylinder during compression is advantageous not only in increasing volumetric efficiency but also in the elimination of undesired combustion process anomalies.

The research investigation program is realized on test engine, produced from the vehicle SI engine type EA111.03D from Škoda Auto Company. The modification of this motor has been made at Department for vehicles and engines on Technical University of Liberec. Detailed description of test engine is stated in [41]. Fuel system for gaseous fuel is based on high pressure injection of gaseous fuel by the special injectors installed on cylinder head with the input of gaseous fuel from the small pressure accumulator (common rail) located at immediacy of injectors.

Fuel system and engine setting parameters are operated, managed and monitored by a special electronic control unit of the ADCIS company where communicates with an engine's operator through a software Monitoring. The software can be controlled by on-line adjustment of basic characteristics (parameters of ignition and fuel injection), for their recording and error diagnostics. Table 4.1 contains the basic parameters of the engine.

Table 4.1: Engine data [41]

PARAMETER	DESCRIPTION, VALUE
Construction	Three-cylinder SI engine
Displacement	1198 cm^3
Bore	76.5 mm
Stroke	86.9 mm
Compression ratio	10.2
Valve train	OHC, 2 valves
Intake pressure [bar]	naturally aspirated engine
Fuel	Hydrogen or natural gas
Cooling	Liquid-cooled engine
ECU	ADCIS

The engine test bench is equipped with a Schenck WT 190 dynamometer. The dynamometer is cooled with water and the temperature regulated by the heat exchanger. Engine heat is also released by the central cooling circuit of the laboratory. Another two heat exchangers located on the motor stand serves to stabilize the temperature range of engine water-cooling and lubricating-oil circuit. The Coramsys software with a graphical user environment is used to collect data and control the dynamometer.

Experimental research have been prepared and conducted at department of vehicles and engines laboratory, Technical University of Liberec. The original 3-cylinder vehicle engine was completely renovated on the fuel system with direct high pressure injection of gaseous fuel (CNG, H_2) to the engine cylinder. To start with, the changes were made on cylinder head to install the high-pressure injector type Hoerbiger Valve Tec. The installation of injectors is shown in Figure 4.1. A general view of the fuel supply to injectors from a rail presently under consideration can be seen in Figure 4.2 and 4.3 show axis geometry of jets injected out of the standard injector nozzle.

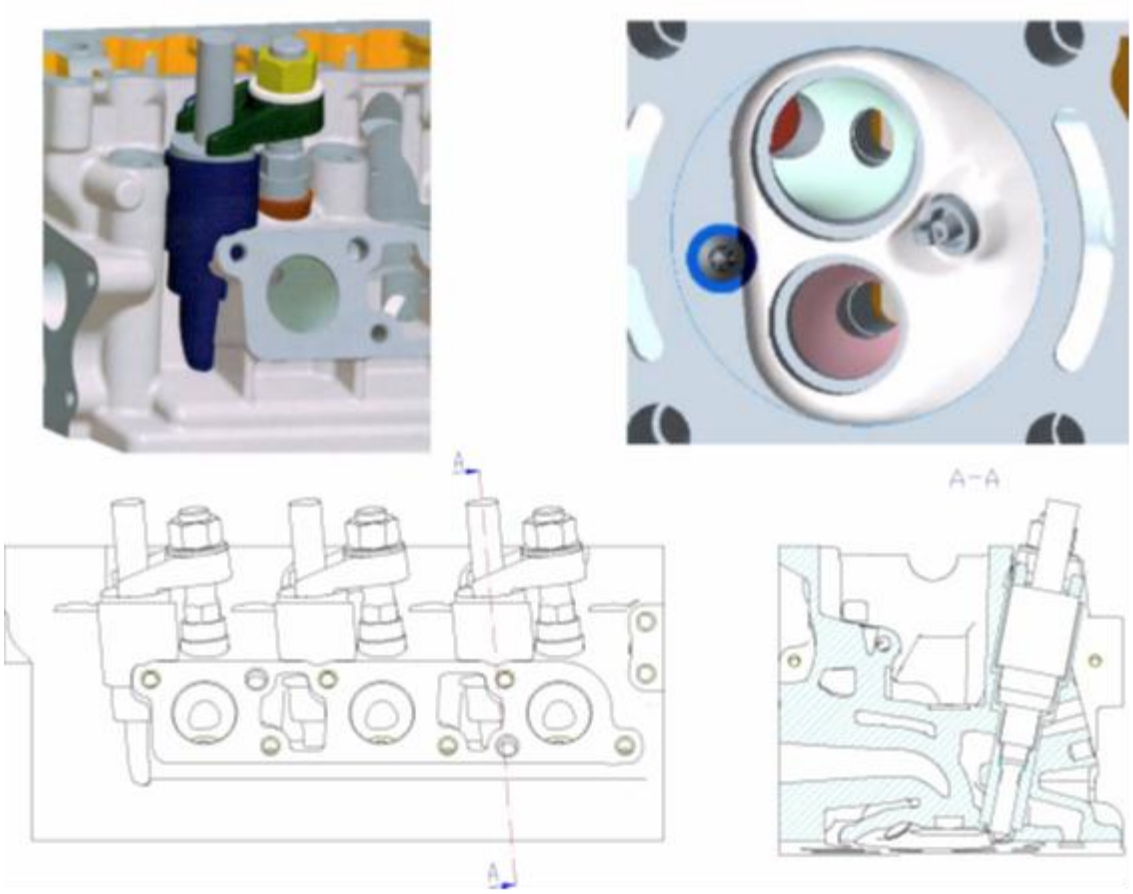


Figure 4.1: Position of a high-pressure gas injector in the internal combustion engine [42]

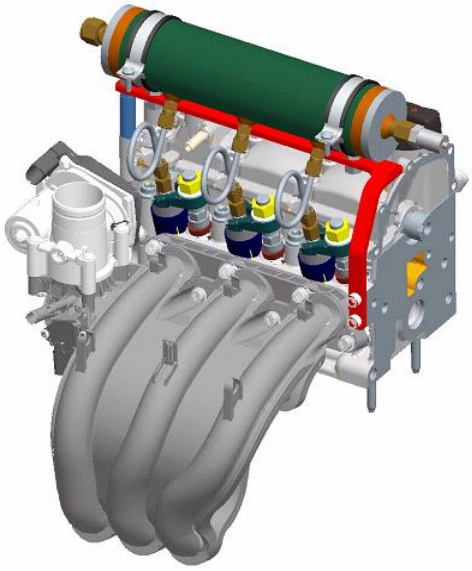
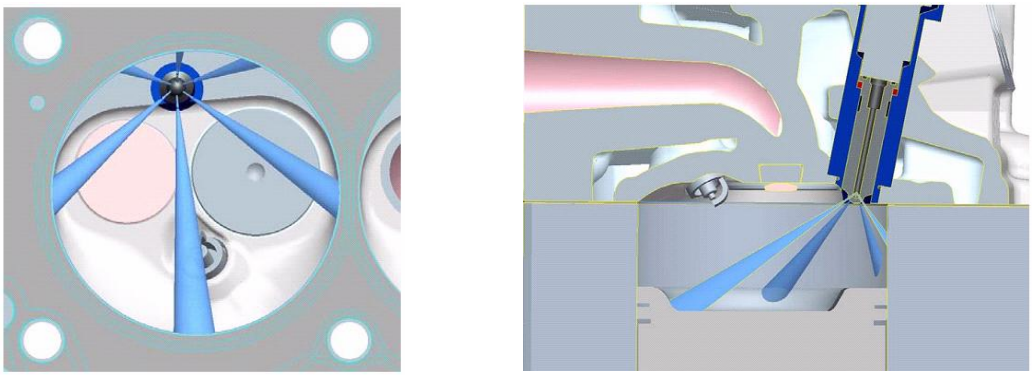


Figure 4.2: View of the fuel supply to injectors from a rail under consideration



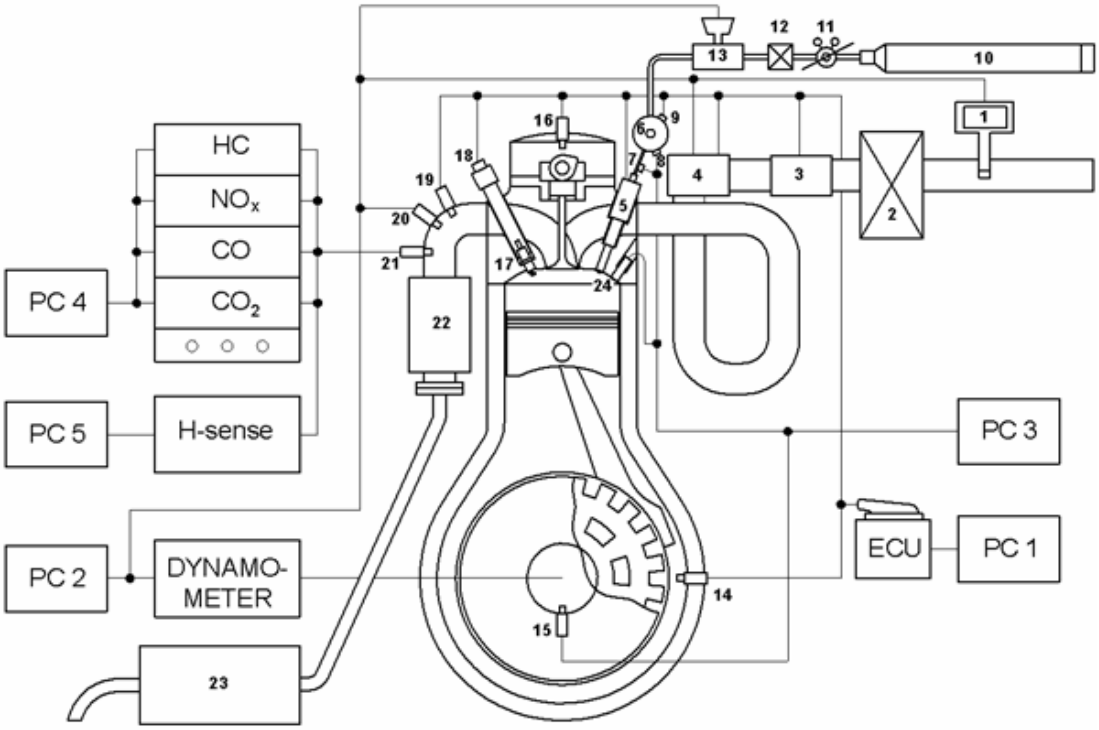
a) b)

Figure 4.3: a) and b) view of axis geometry of jets out of the injector. [42]

The engine concept is based on new high-pressure injectors with 10 MPa inlet pressure. At the moment, our laboratory uses injectors produced by Hoerbiger Valve Tec (the injectors have been developed within the European program HylCE). After being installed in a three-cylinder, 1.2 dm^3 engine, with the hydrogen inlet maximum pressure of 100 bar and the cross-sectional area of flow of 1 mm^2, these high-pressure injectors shorten the injection duration to a maximum 50 degree of the crank angle. Consequently, even at maximum power, the injection can be timed in the compression stroke only after the intake valve closes. The electronic system for the controlling and monitoring of engine operation has been supplied by programmable electronic control unit, ADCIS Company.

4.2 Measurement and control techniques

The test bed is equipped with fully automated data acquisition system for all monitored engine operating variables (standard and specials, including high-pressure indication of the engine working cycle and concentrations of emissions as well as unburned hydrogen in the exhaust gases). Diagram of engine accessories and measurement apparatus is shown in figure 4.4.



1 and **3)** air flow **2)** air filter **4)** throttle **5)** fuel high-pressure injector **6)** fuel rail **7)** fuel pressure sensor before the injector **8)** fuel temperature sensor in the rail **9)** fuel pressure sensor in the rail **10)** fuel reservoir **11)** fuel reduction valve **12)** fuel filter **13)** fuel weight **14) 15)** and **16)** speed and position sensor **17)** spark plug **18)** ignition coil **19)** and **20)** mixing ratio **21)** exhaust gas sample **22)** catalyst **23)** silencer **24)** in-cylinder pressure sensor

Figure 4.4: Schematic of the hydrogen direct injection engine and control system with experimental set-up [41].

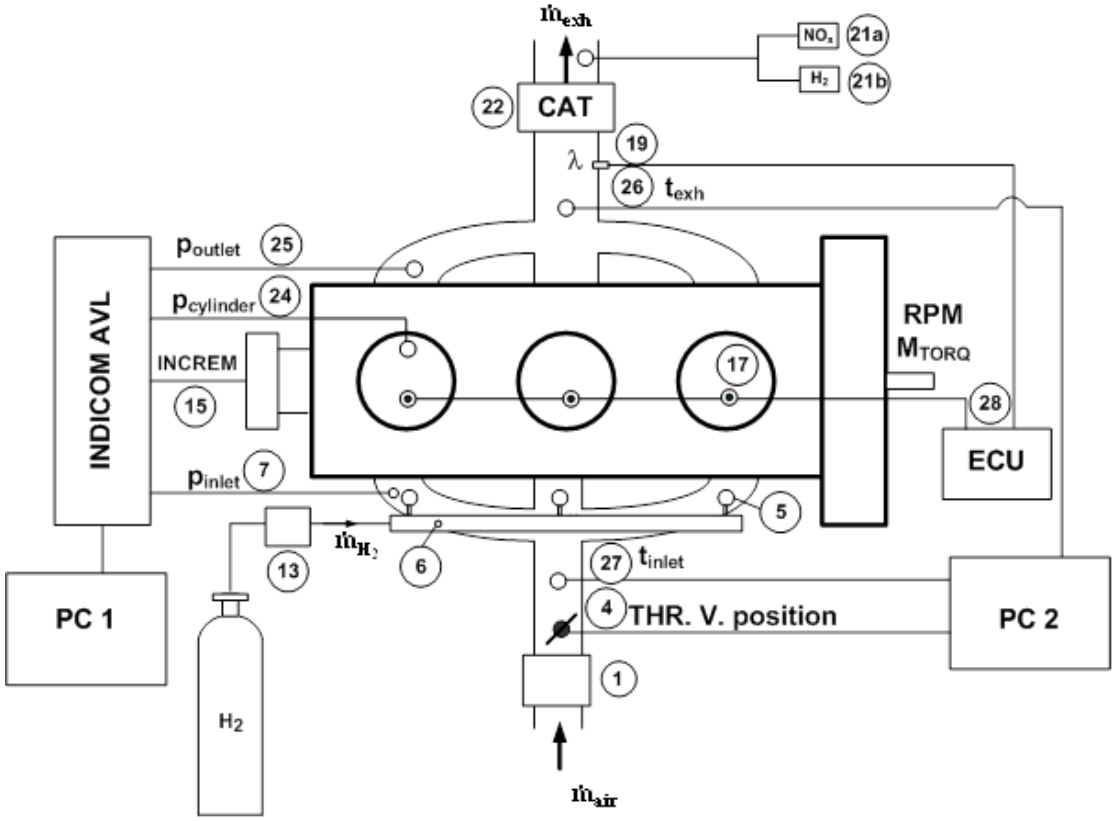


Figure 4.5: Measured arrangement diagram of hydrogen engine

This experiment describes the hydrogen fuel injection arrangements into a cylinder utilized in the laboratory of Technical University of Liberec, Department of Vehicles and Engines. The new workplace for the gas fuelled piston engine with the direct high pressure injection gas to the cylinder was prepared for the research projects MSM: 4674788501, MSM: M0568 (projects MSM with the support from Ministry of Education, Czech Republic) and for the research program of doctoral study.

The research deals with both a low-pressure injector design and a high-pressure injector installation (100 bars) supplied by a specialized producer. Figure 4.5 indicates a layout of experimental three-cylinder engine with ECU accessories for mixture forming using direct injection of hydrogen to cylinder engine. In addition, the details of measured devices are provided in Table 4.2.

Table 4.2: list of measured device system

Item	Description	Product
1	Air flow meter	SIERRA Instrumentation, inc. 2500 l/min, 150 psig
4	Position sensor/ Throttle valve	SIEMENS VDO serial 03D133062E
5	Injector	Hoerbiger Valve Tec
6	High pressure fuel system (common rail)	Designed by Dept. Motor & Vehicle, TUL
7	Fuel pressure sensor before injector	AVL GU21D/ KULITE ETM-3752 / 2500 PSI
13	Fuel flow meter	Micro Motion inc. /Elite CMF 2700
15	Speed and position sensor	LARM a.s. Netolice/IRC315 0-60 ^{o}C, 10,000 1/min
17	Spark plug	BRISK Silver DR12YS
19	Lambda sensor	SKODA-036906262G
21a	NO_x emission Analyzer	HORIBA Chemiluminescent analyzer
21b	H_2 exhaust indicator	H-SENSE: V&F Analyses und Messtechnik Serial 0610167/220-240v
22	Catalytic converter	SKODA 03D 131 701G
24	In-cylinder pressure sensor	AVL GU21D
25	Exhaust pressure sensor	AVL GU21D
26	Exhaust temperature sensor	NiCr-Ni JHCH 0336
27	Intake air temperature/ Pressure sensor	MAPS 03D906051
28	Electronic control unit (ECU)	ADCIS a.s. company

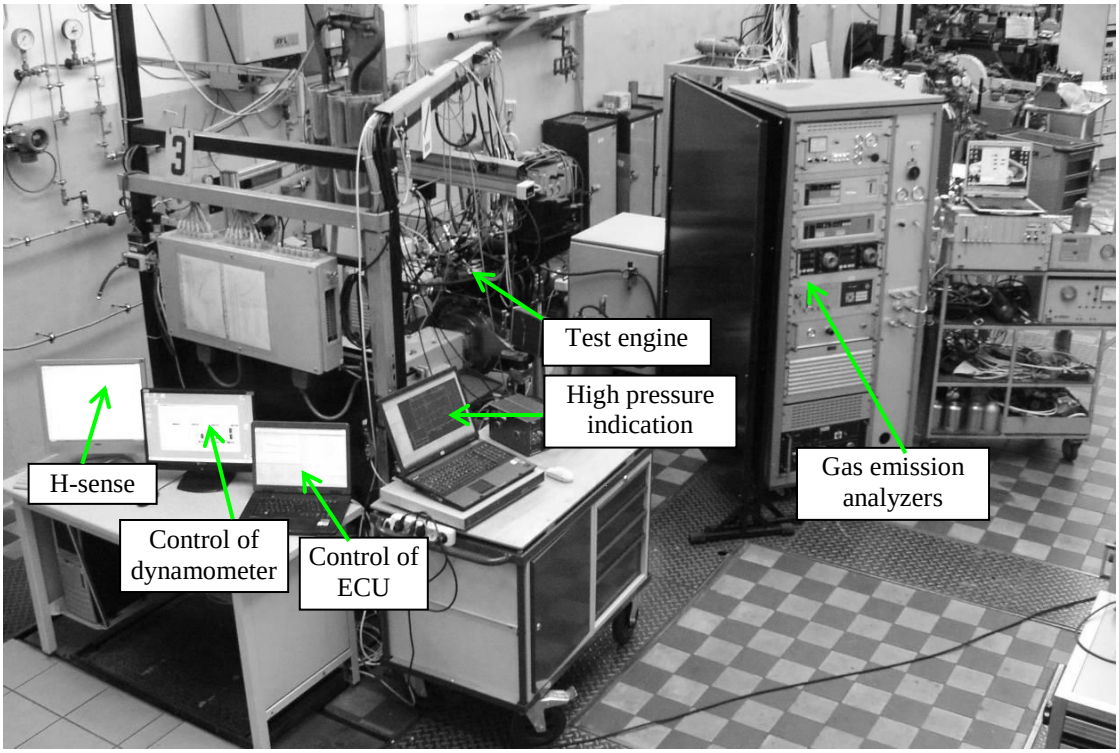


Figure 4.6: Test engine and experimental apparatus [41]

4.3 Experimental program on testing engine

High pressure injection of gaseous fuel there is timing to the compression stroke of piston with the start of injection to the position of crank angle near cutting-off inlet valve. Original (serial) and modified engine they have identical cam-shaft, which wholly close the inlet valve till in position 111°BTDC (i. e. at advanced state of the compression stroke – timing of inlet valve is optimized for on utilize of wave effect in suction manifold for the good filling of cylinder engine.

According to formerly performed measuring it was decision to move the start of fuel injection further before TDC for the increasing of mixture forming time (for reaching of good homogeneity mixtures). Unclosing of inlet valve, at which already no-threatens dangerous outflow of the injected gaseous fuel (mixtures) by backward flow into sucking tract was assessed in value 0.2-0.3 mm of the inlet valve lift. Thereby them it is excluded the further ignition of fresh mixtures in suction tract by very hot product of combustion. Start of injection of gaseous fuel to the cylinder engine will, according to those thinking, located on position 140-130 °BTDC.

At next figure there are plotted the course of cylinder pressure and the courses of the lifting characteristic of the inlet and exhaust valve. The safety lift limit 0.3 mm for inlet valve there is showed also.

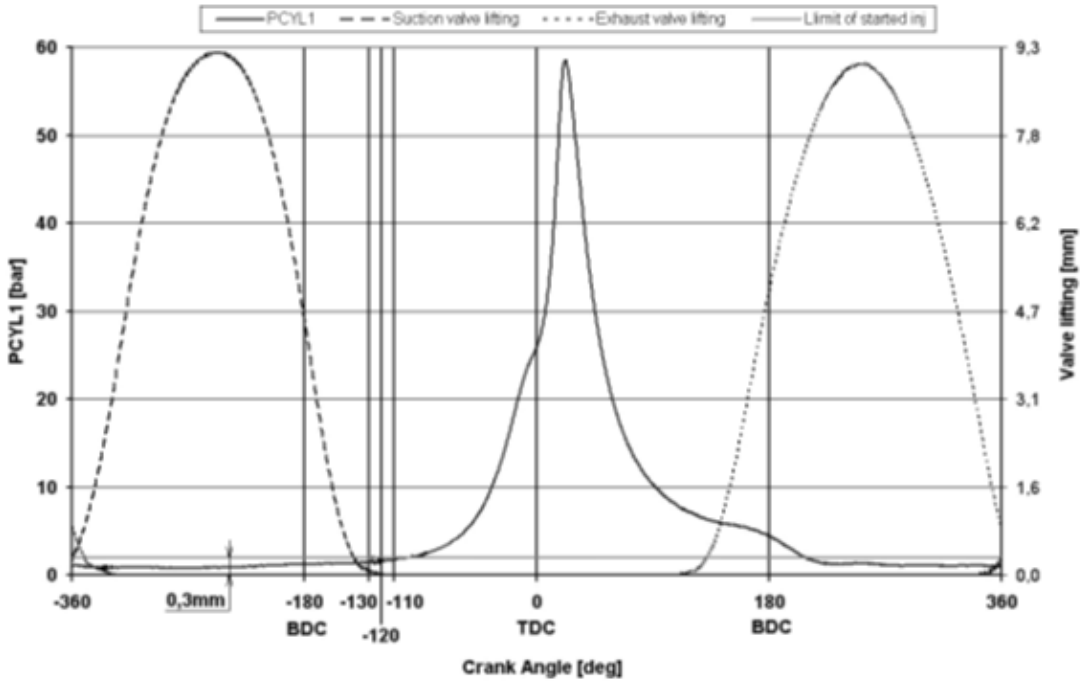


Figure 4.7: The course of cylinder pressure and lifting characteristic for the inlet and exhaust valve. [43]

Modified gas (CNG, H_2) engine for the direct high pressure injection of gaseous fuel (common rail system) to cylinder engine was located on test bench at laboratory of Department vehicle and engine, Technical University of Liberec. Test bench is facilities by fully automated (electronically controlled) system of data collection for all watched operational quantity of engine (common and above standard quantities, including high pressure indication of working cycle of engine and measurement system for the concentration of gaseous harmful components in exhaust gases also).

Engine was equipped by special ECU from the Czech company ADCIS with the control software Monitor 3. The experimental research program was started after full activation of engine with progressive adjustment of all systems at the test bench. Within the frame of doctoral study the experiments were performed with hand control of ECU (the position of throttle valve, injection pressure of gaseous fuel, start of fuel injection, duration of fuel injection - fuel charge, advance of spark ignition). Experimental program for doctoral study was aimed to research of engine behavior on H_2 running. Start and warming-up of engine was performed on CNG. The results and experiences from this measuring were determined for the formation of program (tables) for the master adjusting of engine characteristics. The preparing plan of the measurement for Hydrogen fuelled engine fuelled engine is indicated on table 4.3.

Table 4.3: Plan of measuring, the variability of the setting parameters of the hydrogen fuelled internal combustion engine

Parameter	Speed	Fuel pressure	Start of injection	Spark advance	λ
Unit	[1/min]	[bar]	[^{o} BTDC]	[^{o} BTDC]	[-]
Setting up ECU	(2000) 3000 (4000)	50	110 120 130	5 15	1.8 2.0 2.2
		75	110 120 130	5 15	1.8 2.0 2.2
		100	110 120 130	5 15	1.8 2.0 2.2

The first part of experimental on engine fuelled Hydrogen engine was set on investigation of influence of fuel injection pressure (p_{inj}) of 50, 75 and 100 bar, start of injection (SOI) at 110, 120 and 130 ^{o} BTDC, ignition timing (α_{IGN}) of 5 and 15 ^{o} BTDC and richness of mixture (λ) from 1.8 to 2.2 on characteristics of working cycle, course of combustion and content of NO_x, O_2 and H_2 in exhaust gases. All measured parameters were recorded at mode of load characteristic on engine speed of 3000 1/min.

4.4 Evaluation of measured data

This section describes the basics of engine parameters measurements, monitoring and evaluation, most importantly, the applied formulas and calculation methods. All measured data from experiment will be collected and evaluated by AVL Indicom then they are analyzed, verified and presented by Concerto software. The AVL applied the statistic and numerical method for access all data as the following section. The pressure signal amplified by a charge amplifier is fed to the data acquisition linked to a personal computer. An AVL acquisition program is used to sample and store the pressure data fed to data acquisition. The AVL sampling program has been written to collect 150 consecutive engine cycles.

Indicated mean effective pressure

In the four-stroke engine the indicated mean effective pressure corresponds to the total of the area integrals of both loops of the p-V diagram. On the p-V diagram, mean indicated pressure can be determined by the following definition

$$\mathbf{p_i} = \frac{1}{\mathbf{V_S}} \int_{-360}^{+360} \mathbf{p}\, \mathbf{dV} \quad , \tag{4.1}$$

where V_s is swept volume.

Rate of Heat Release

A simplified process is used to calculate the heat release which computes the energy effectively delivered to the gas from the cylinder pressure. Surface losses (approx. 20%) are neglected; the displayed heat release is therefore accordingly lower than the actual energy released. The calculation is based on the first law of thermodynamics.

The software, IndiCom Application, uses the first law of thermodynamics for calculating the rate of heat release in real time

$$\mathbf{Q_i} = \frac{\mathbf{K}}{\boldsymbol{\kappa} - 1}\left[\boldsymbol{\kappa} \cdot \mathbf{p_i}(\mathbf{V_{i+1}} - \mathbf{V_{i-n}}) + \mathbf{V_i} \cdot (\mathbf{p_{i+n}} - \mathbf{p_{i-n}})\right], \tag{4.2}$$

where n interval (1 degree CA),
κ polytropic coefficient, for SI engine the value κ = 1.35,
p cylinder pressure,
V volume,
K constant (100...due to unit conversion).

Coefficient of Variability (VAR)

Spark ignition engines are characterized by wide variability of mixture combustion development (significant fluctuation of p_{max} as well as α_{COMB}).

A variability of Mean Indicated Pressure (VAR_{pi}) is a commonly accepted variable for combustion stability and is one of possibilities for estimation of stability of mixture burning in cylinder. Change of in-cylinder pressure shapes among recorded indicator diagrams is marked as variability among cycles and it can be calculated using Coefficient of Variability (VAR) or Variability of cycles. VAR is a global indication of engine stability is usually interpreted as the ratio of mean indicated pressure standard deviation to average value of mean indicated pressure in given operating mode, expressed as equation (4.3).

$$\mathbf{VAR_{P_i}} = \frac{\overline{\boldsymbol{\sigma}}_{\mathbf{p_i}}}{\overline{\mathbf{p}}_{\mathbf{i}}}.100 \quad [\%], \tag{4.3}$$

where $\overline{\boldsymbol{\sigma}}_{\mathbf{pi}}$ is a Standard deviation of mean indicated pressure from statistical processing of indicator diagrams set, it can be evaluated by equation (4.4),

$\overline{\mathbf{p}}_{\mathbf{i}}$ is arithmetic mean of indicated pressure of recorded indicator diagrams, over a number of consecutive combustion cycle. In the performed experiments, 150 combustion cycles were used for calculating each estimate, as equation (4.5).

$$\overline{\boldsymbol{\sigma}}\mathbf{p_i} = \sqrt{\frac{\sum_{\mathbf{i}=1}^{150}(\overline{\mathbf{p}}_{\mathbf{i}} - \mathbf{p_i})^2}{150 - 1}} \tag{4.4}$$

$$\overline{\mathbf{p}}_{\mathbf{i}} = \sum_{1}^{150}\mathbf{p_i} \tag{4.5}$$

The additional possibility for appreciation of stability of mixture burning in cylinder is a variability of maximal in-cylinder pressure (p_{MAX}) among recorded indicator diagrams. It can be calculated using equation (4.6).

$$\mathbf{VAR\ p}_{max} = \frac{\boldsymbol{\sigma}_{\mathbf{p_{MAX}}}}{\bar{\mathbf{p}}_{\mathbf{MAX}}}.100 \qquad [\%] \qquad (4.6)$$

,

where $\boldsymbol{\sigma}_{\mathbf{p_{MAX}}}$ is a standard deviation of p_{MAX} values of recorded indicator diagram That it can be found in equation (4.7),

$\bar{\mathbf{p}}_{\mathbf{MAX}}$ is arithmetic mean of p_{MAX} of recorded indicator diagrams.

$$\boldsymbol{\sigma}\mathbf{p}_{\mathbf{MAX}} = \sqrt{\frac{\sum_{\mathbf{i}=1}^{150}(\bar{\mathbf{p}}_{\mathbf{MAX}} - \mathbf{p}_{(\mathbf{MAX})\mathbf{i}})^2}{150-1}} \qquad (4.7)$$

Exhaust emission measurement devices

The method of monitoring gas engine emissions is continuous measurement of NO_x and unburned hydrogen. Exhaust gaseous emissions analyzers use electrochemical sensors to measure NO_x. Measurement of NO_x during research will typically be performed using a more sophisticated chemiluminescent detector. The meter measures the amount of light emitted by photons released when nitrogen oxide reacts with ozone. The sample passes through a catalyst to convert any NO_2 to NO and then is exposed to ozone. The intensity of the ensuing reaction is proportional to the amount of NO in the sample. This meter requires water to be removed from the sample; hence, the results will be expressed as dry.

Unburned hydrogen content in emission is typically measured using a mass spectrometer analyzer [H-sense]. The analyzer is controlled and monitored by a PC and the sample is required in dry basis.

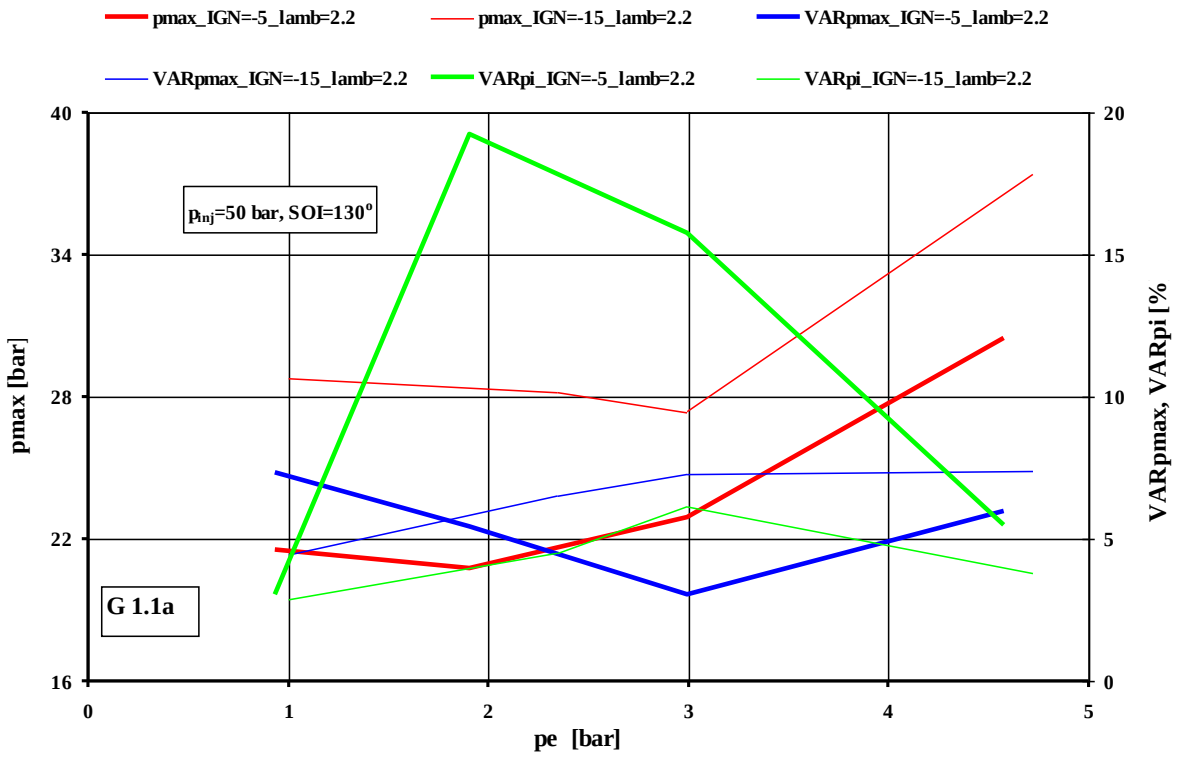
The tests were performed at the Engines Laboratory of the Technical University of Liberec. The experimental unit consists of engine test, dynamometer, controllable ECU, exhaust emission analyzers, combustion process monitoring unit. To make sure an accuracy of the emission level, the emission analyzers were always calibrated before the experiment began. In addition, the exhausts gaseous were treated before leaving to surroundings. The engine parameters, for example, mean indicated pressure, maximum pressure in cylinder and unburned hydrogen as well, were monitored, analyzed and recorded by software of AVL while level of emission content such as unburned hydrogen and NO_x parameter were recorded with Indicom software. The Coramsys software with a graphical user environment is used to collect data and control the dynamometer. Finally, the Concerto is a tool that developed by AVL were used to evaluated all engine data and presented by many graphs where are displayed in Appendix 1.

CHAPTER 5

RESULTS AND DISCUSSION

Introduction

Big set of the measurement was fulfillment on the experimental hydrogen engine with the direct high pressure injection of the gaseous hydrogen to the cylinder engine. Results argue that the conception of SI hydrogen engine with the internal mixture formation has a good background for the next research work on automotive engine for the absolutely renewable fuel. The measurement, elaboration and evaluation of the results however shows at the same time, that for the achievement of the useful quality of the hydrogen automotive engine will need the next sophisticated (temporal and financially) research and development for solution of the rows of technically complicated problems. Following selection of the results from performed measurement documents how positive, so problematic properties, recognized on experimental hydrogen engine.



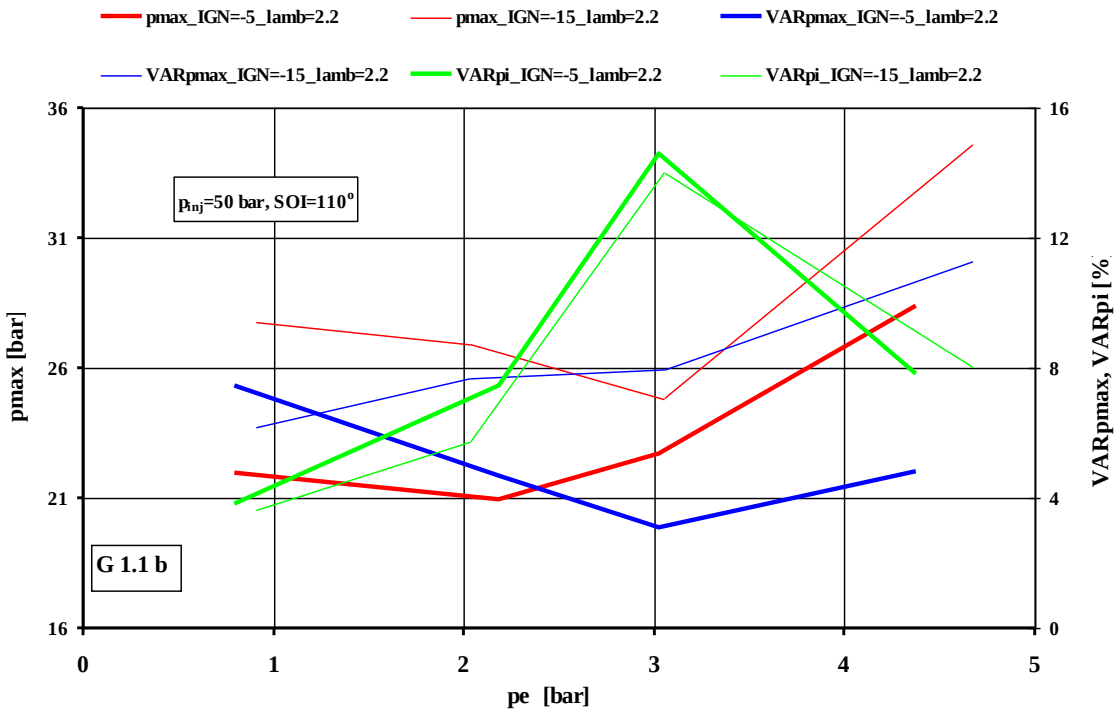
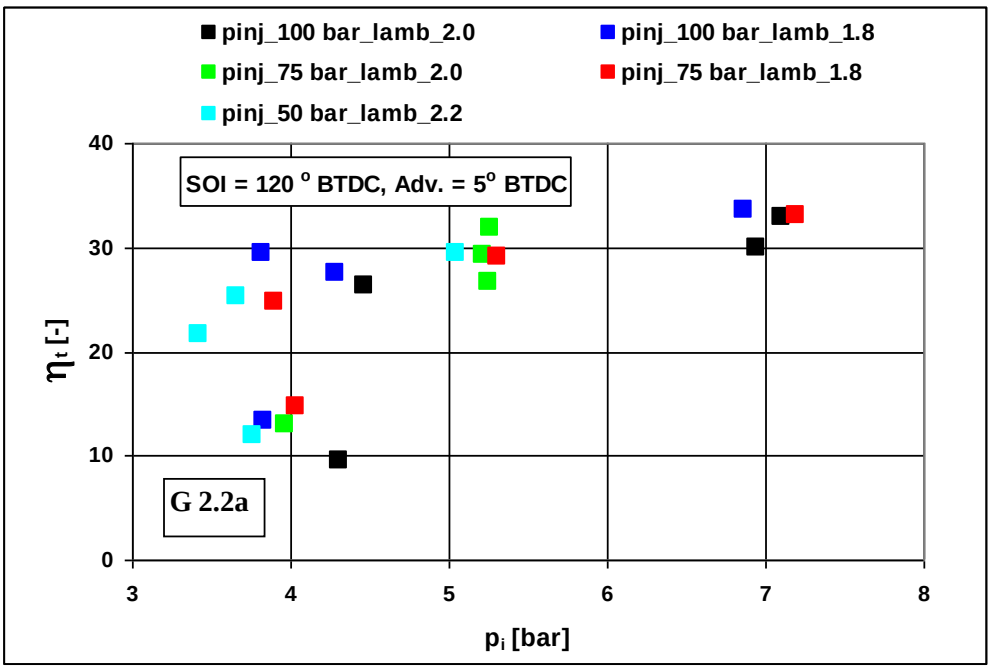


Figure G 1.1 a) and b)

Figure G 1.1 a) and b) show the essentials parameters of the working cycle of the hydrogen experimental engine for the engine speed at 3000 1/min and the marked setting. The values of the p_{max} are harmony both to load and setting-up of engine. The variation of the maximum pressure (p_{max}), coefficient of variability in p_{max} (VAR_{pmax}) and mean indicated pressure (VAR_{pi}) have a relative big value (in comparison to standard SI vehicle engines) – it is probably the consequence to high inhomogeneity of the internal forming mixture.

It can be observed that the increases of p_{max} with increases in the p_e and starting of injection time(standard quality). At lean condition (λ=2) with low load of engine results in higher maximum cylinder pressure (p_{max}). Higher unstability of p_i and p_{max} course in cylinder occur within mean effective pressure range (1-4 bar) at lambda of 1.8 and starting ignition of 5 ^{o}BTDC. The effects of the starting injection time on maximum cylinder pressure with p_e are not significant. The graphic elaboration of the other results (p_{max}, VAR_{pmax}, VAR_{pi}) from the measuring at group of graphs G1 they show to the similar conclusion.



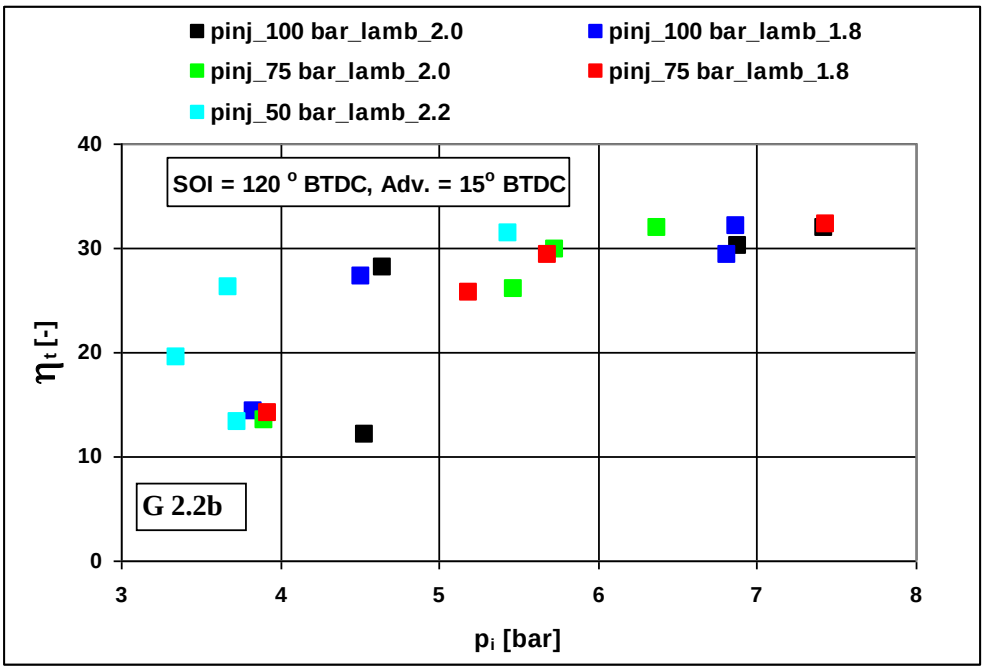


Figure G 2.2 a) and G 2.2b)

The graphs display total efficiency (η_t) versus mean indicated pressure (p_i) at 3000 1/min, spark advance of 5° BTDC (15° BTDC) and starting of injection at 120° BTDC on various fuel injection pressure (p_{inj}) and excess air ratio.

As can be seen from figure G 2.2 a) and b), the values of total efficiency of hydrogen engine they are very near to standard SI vehicle engine – the high dispersion of this values it can be effect of the high variability of working cycle parameters. At lower pressure of fuel injection and lean condition, the influences of injection pressure and air excess ratio are not substantial.

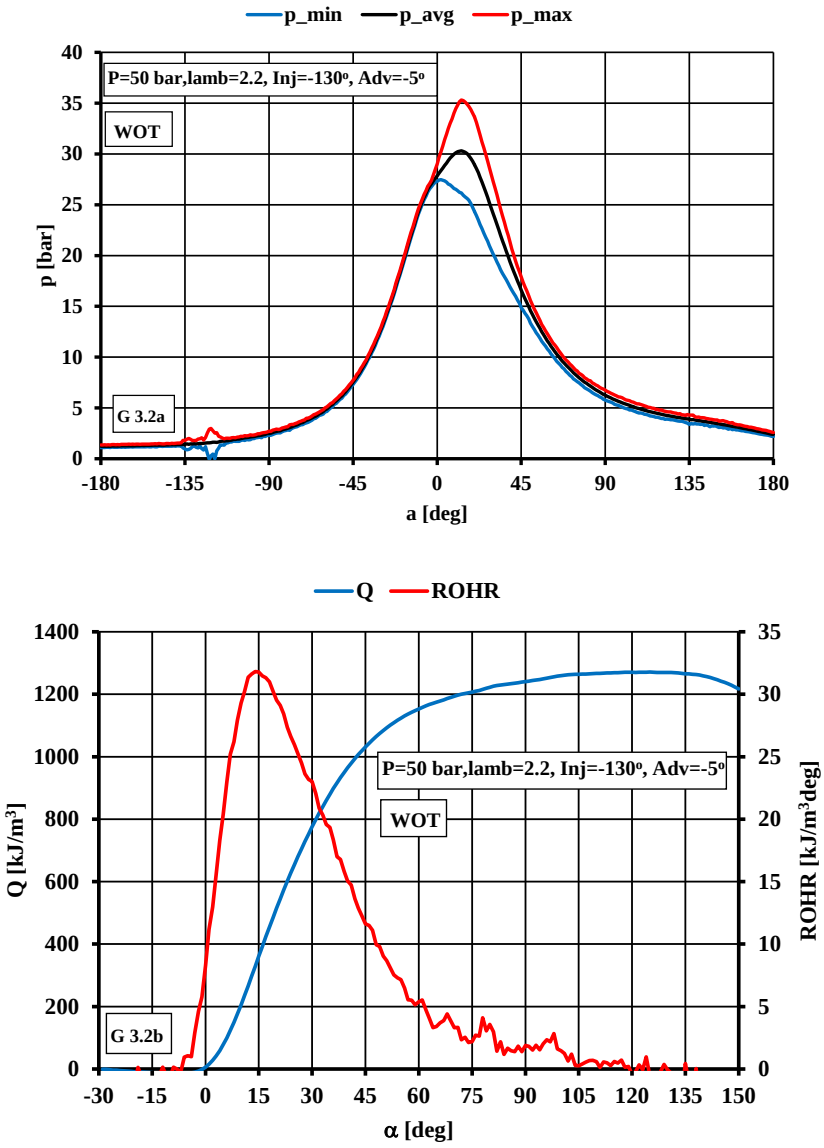


Figure G 3.2a and 3.2b

The variation of the courses of cylinder pressure (lines for the cycle with the average value of the mean indicated pressure, for maximum value of p_i and minimum value of p_i) at 100% load (WOT) and 3000 1/min at marked setting-up of hydrogen engine. Heat of combustion and rate of heat release (ROHR) on angle of crankshaft there is draw for the cycle with the average value of the mean indicated pressure for the marked regime of engine.

It is clearly to perceive from the figure that there is almost no delay on the start of combustion. The high burning velocity of hydrogen decreases the engine combustion duration which is helpful on reducing time of combustion delay. The course of the burning of hydrogen-air mixture has 2 phases – duration of the main phase is about 60 – 70 degree CA (raw estimation), total duration of the burning can be 120 degree CA. It probably has the relationship to inhomogenity of the mixture.

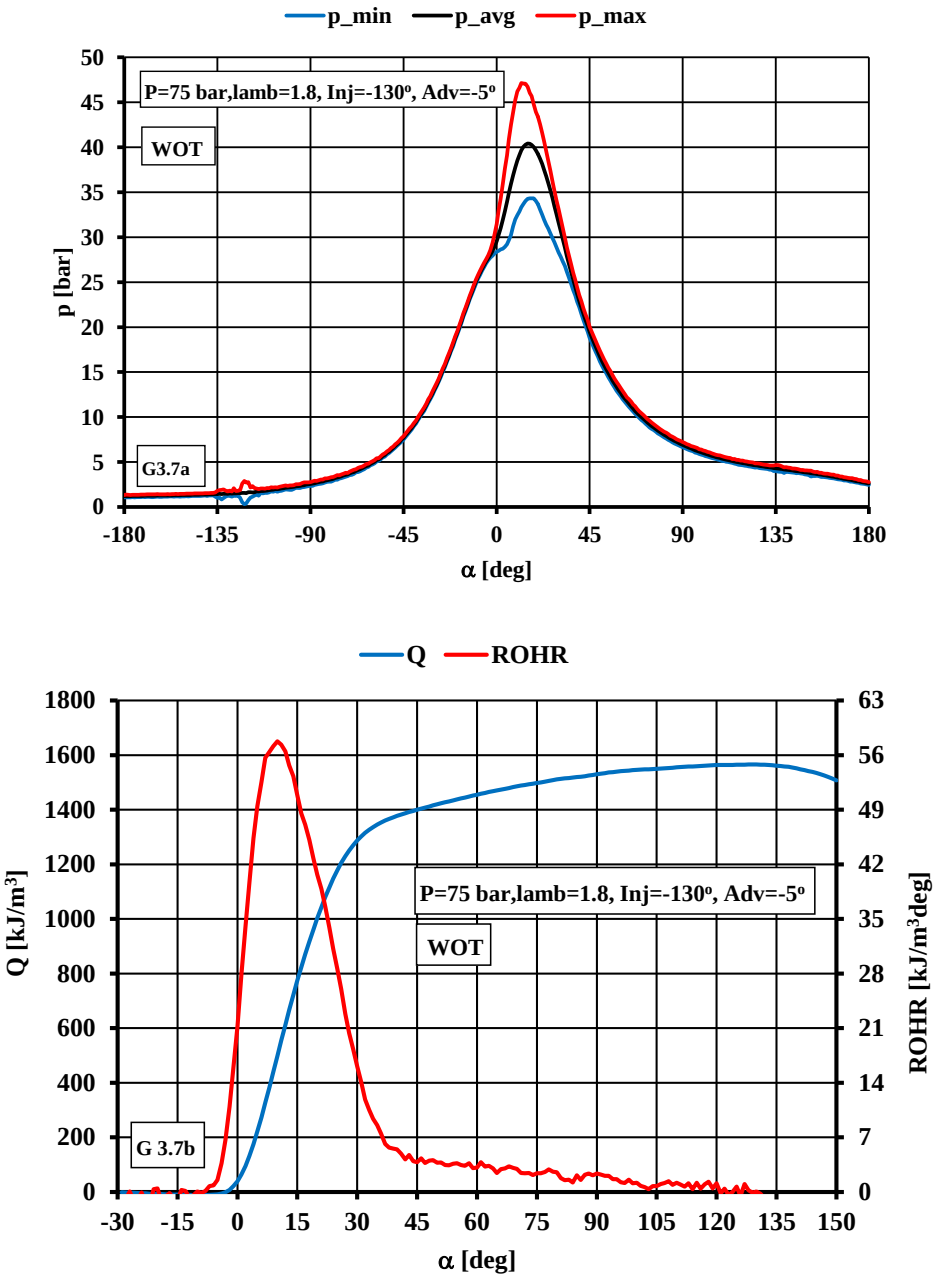


Figure G 3.7a and 3.7b

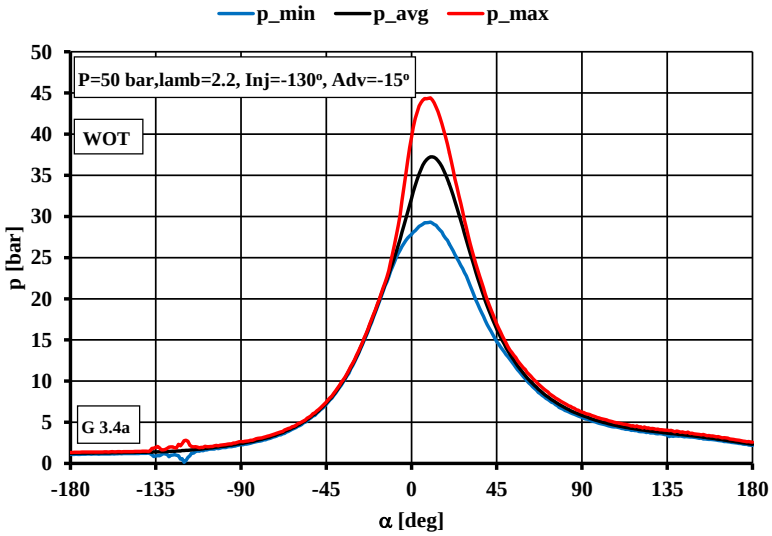
The variation of the courses of cylinder pressure (lines for the cycle with the average value of the mean indicated pressure, for maximum value of p_i and minimum value of p_i) at 100% load (WOT) and 3000 1/min at marked setting-up of hydrogen engine. Heat of combustion and rate of heat release (ROHR) on angle of crankshaft there is draw for the cycle with the average value of the mean indicated pressure for the marked regime of engine.

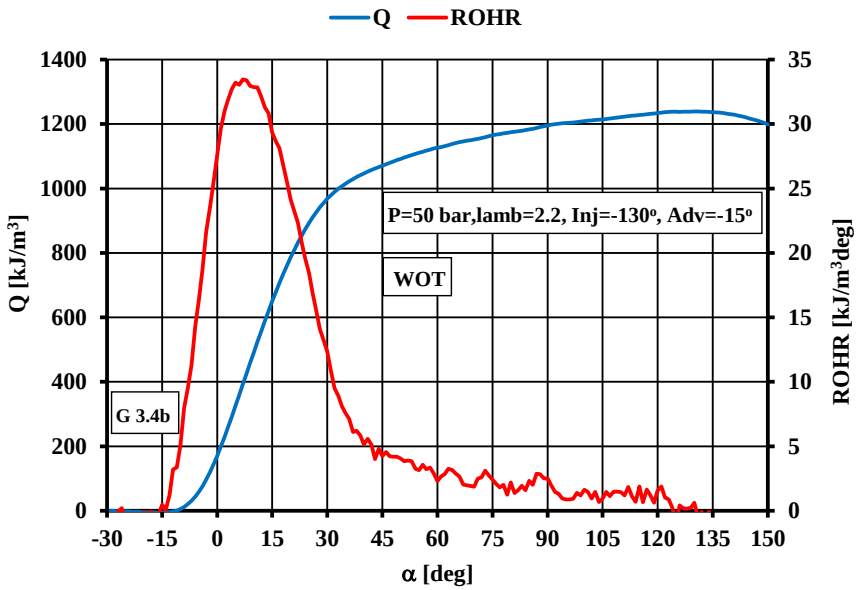
It is clearly to see from the figure that there is a little delay on the start of combustion. The high burning velocity of hydrogen decreases the engine combustion duration which is helpful on reducing time of combustion delay. The higher pressure of injection (75 bar) can produce higher pressure in cylinder compared to the injection pressure of 50 bar, consequently, lead to faster release the heat of combustion.

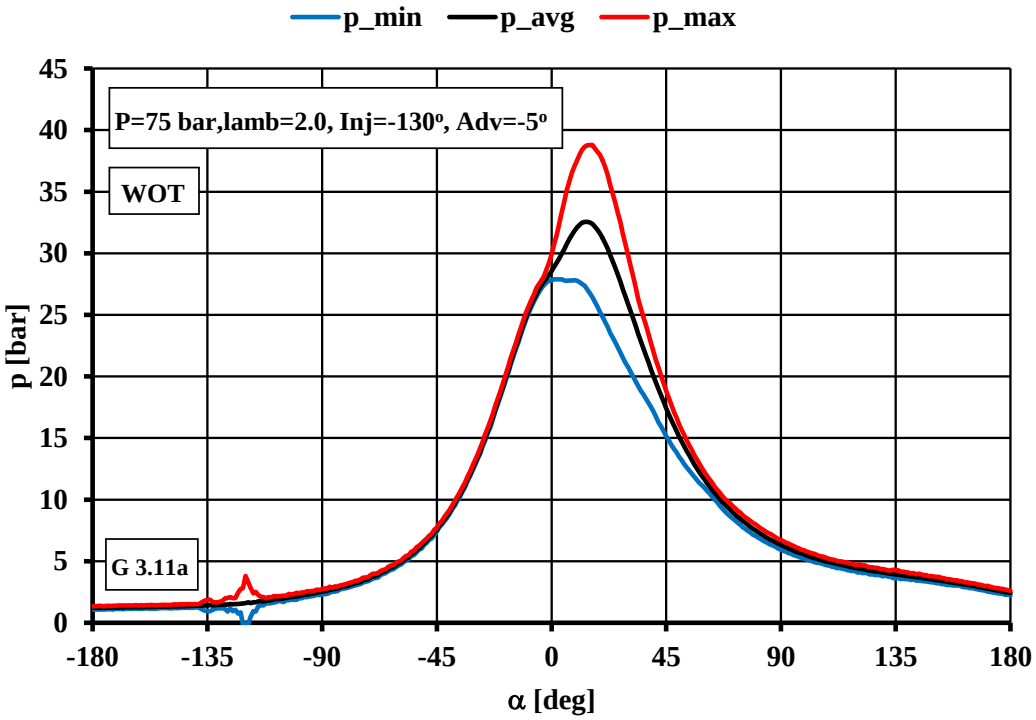
Figure G 3.4 and 3.11

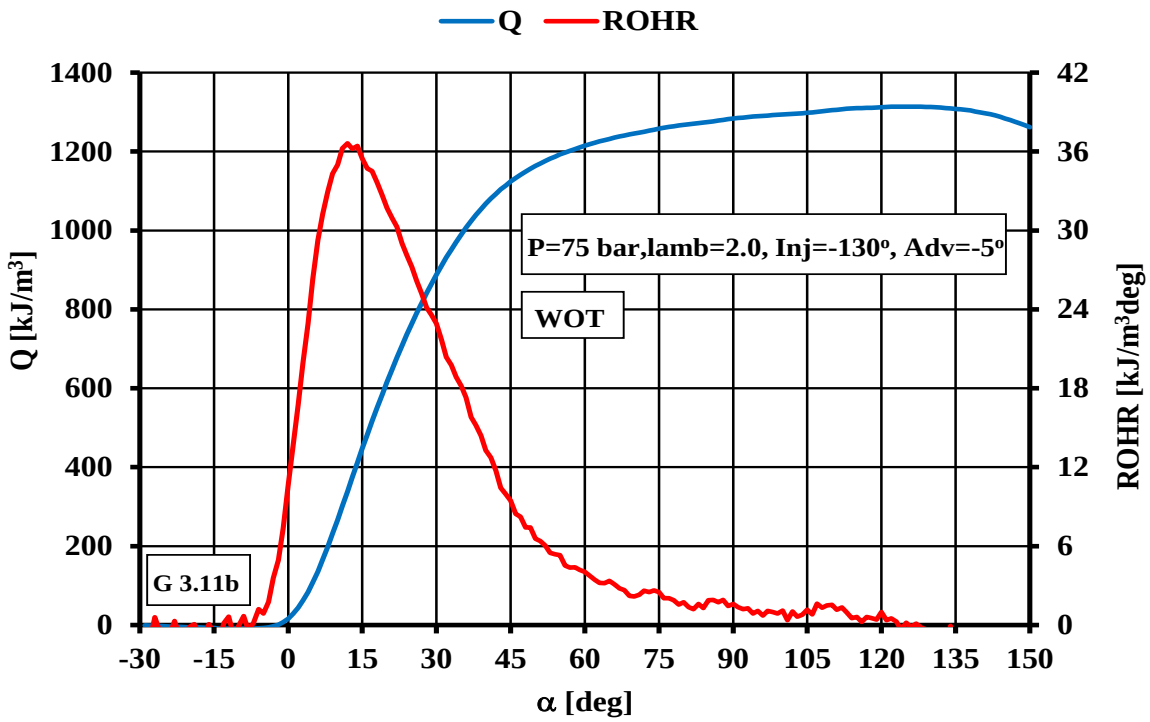
The variation of the courses of cylinder pressure (lines for the cycle with the average value of the mean indicated pressure, for maximum value of p_i and minimum value of p_i) at 100% load (WOT) and 3000 1/min at marked setting-up of hydrogen engine. Heat of combustion and rate of heat release (ROHR) on angle of crankshaft there is drew for the cycle with the average value of the mean indicated pressure for the marked regime of engine.

It is clearly to perceive from the figure that there is a little delay on the start of combustion (practically zero delay of ignition). The high burning velocity of hydrogen decreases the engine combustion duration which is helpful on reducing time of combustion delay. The course of the burning of hydrogen-air mixture has 2 phase – duration of the main phase is about 60 – 70 deg.CA (raw estimation), total duration of the burning can be 120 deg.CA. It has (probably) the relationship to inhomogeneity of the mixture.






p_min
p_avg
p_max
P=75 bar,lamb=2.0, Inj=-130º, Adv=-5º
WOT
G 3.11a
p [bar]
α [deg]
45
40
35
30
25
20
15
10
5
0
-180
-135
-90
-45
0
45
90
135
180


Q
ROHR
P=75 bar,lamb=2.0, Inj=-130º, Adv=-5º
WOT
G 3.11b
Q [kJ/m3]
ROHR [kJ/m3deg]
α [deg]
1400
1200
1000
800
600
400
200
0
42
36
30
24
18
12
6
0
-30
-15
0
15
30
45
60
75
90
105
120
135
150

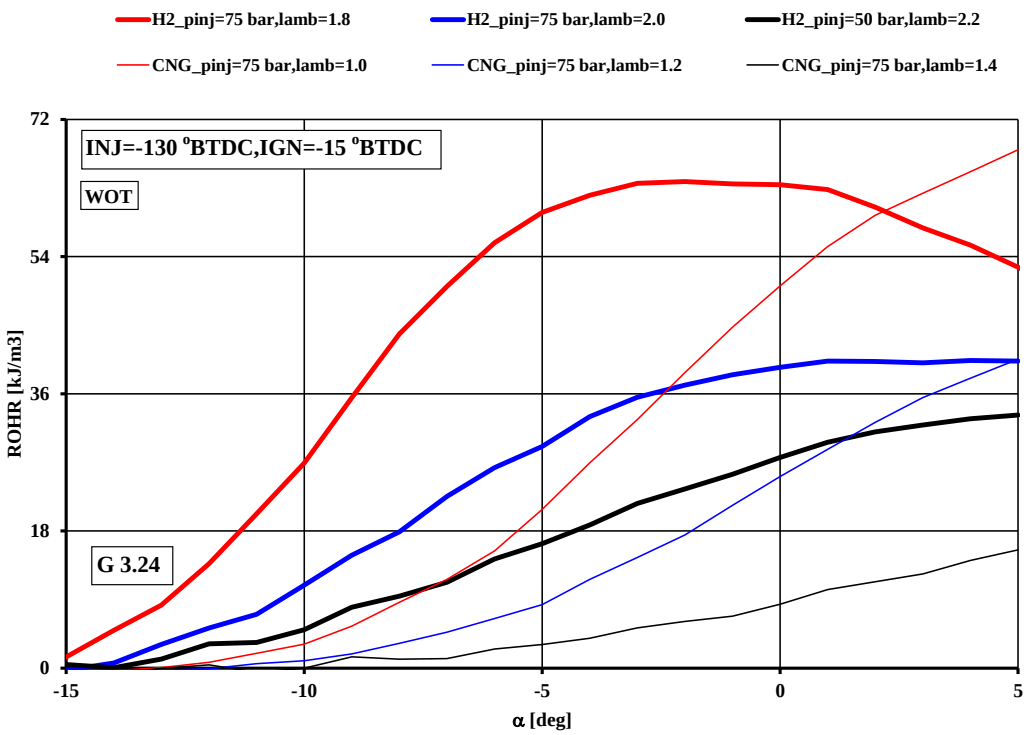
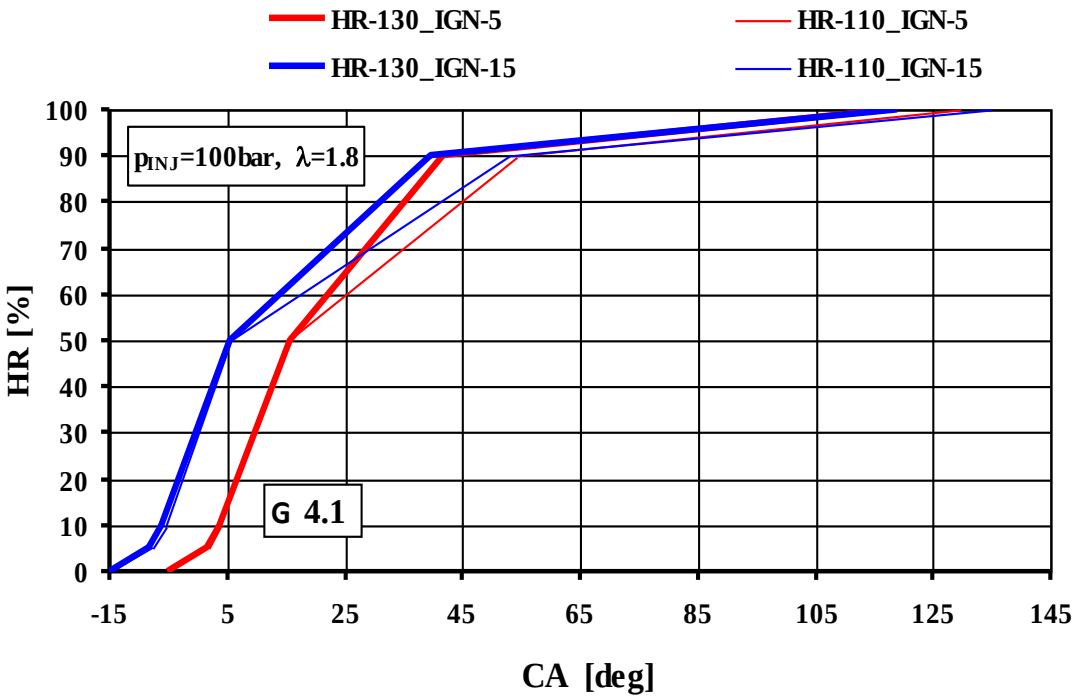
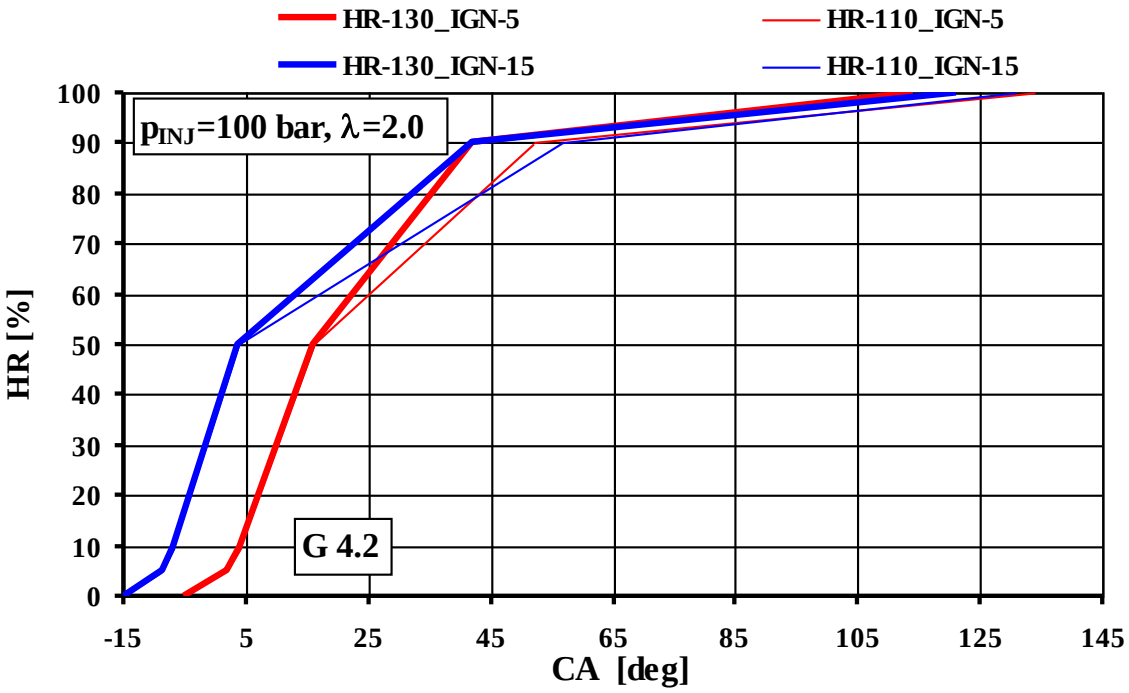


Figure G 3.24

Figure G 3.24 indicates the variation of rate of heat release (ROHR) on crank angle (degree) at 3000 rpm and WOT for hydrogen and CNG at the initial phase of the burning. The setting-up of the experimental engine there was the same considering to the spark advance and injection fuel timing, but different regarding to air excess ratio (λ).

The courses of the ROHR show that the combustion of hydrogen will start more rapidly (with the zero ignition delay) compared with CNG do. This is a good characteristic of hydrogen. At lower air excess ratio (λ) with the same injection pressure, higher rate of heat release for hydrogen can be noticed compared with CNG. Also, heat of combustion will release more rapidly for lower value of λ both hydrogen and CNG. The very good ignitability of the hydrogen-air mixture they are at very low of the load engine. It shows on the next graphs.


HR-130_IGN-5
HR-110_IGN-5
HR-130_IGN-15
HR-110_IGN-15
pINJ=100bar, λ=1.8
G 4.1
HR [%]
CA [deg]
100
90
80
70
60
50
40
30
20
10
0
-15
5
25
45
65
85
105
125
145


HR-130_IGN-5
HR-110_IGN-5
HR-130_IGN-15
HR-110_IGN-15
pINJ=100 bar, λ=2.0
G 4.2
HR [%]
CA [deg]
100
90
80
70
60
50
40
30
20
10
0
-15
5
25
45
65
85
105
125
145

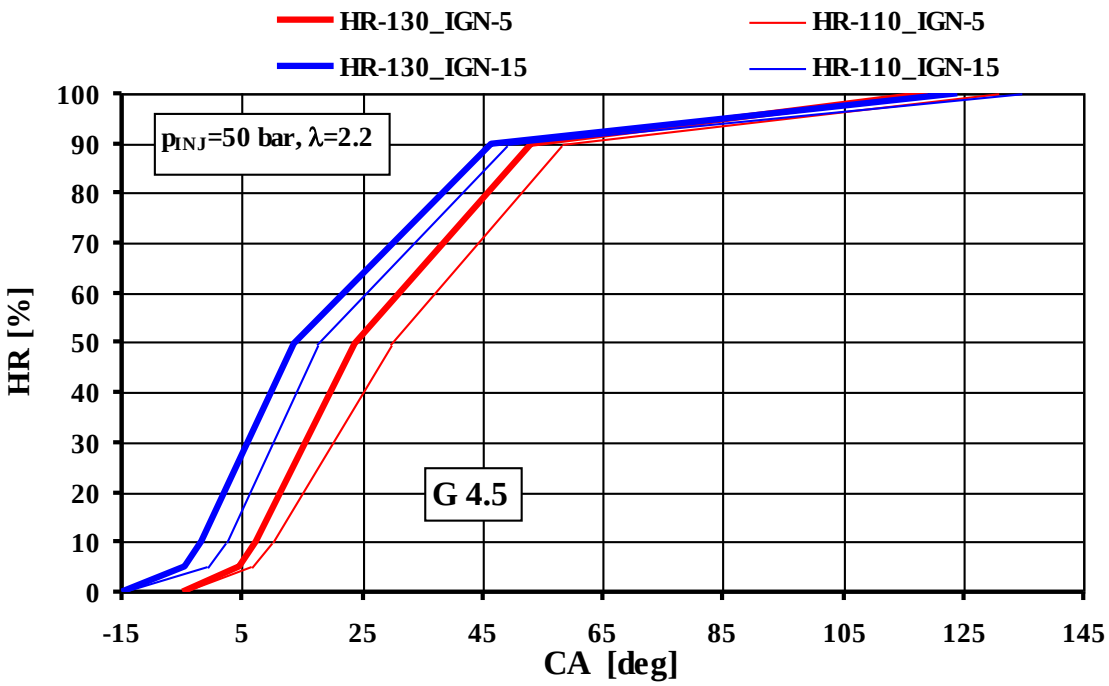
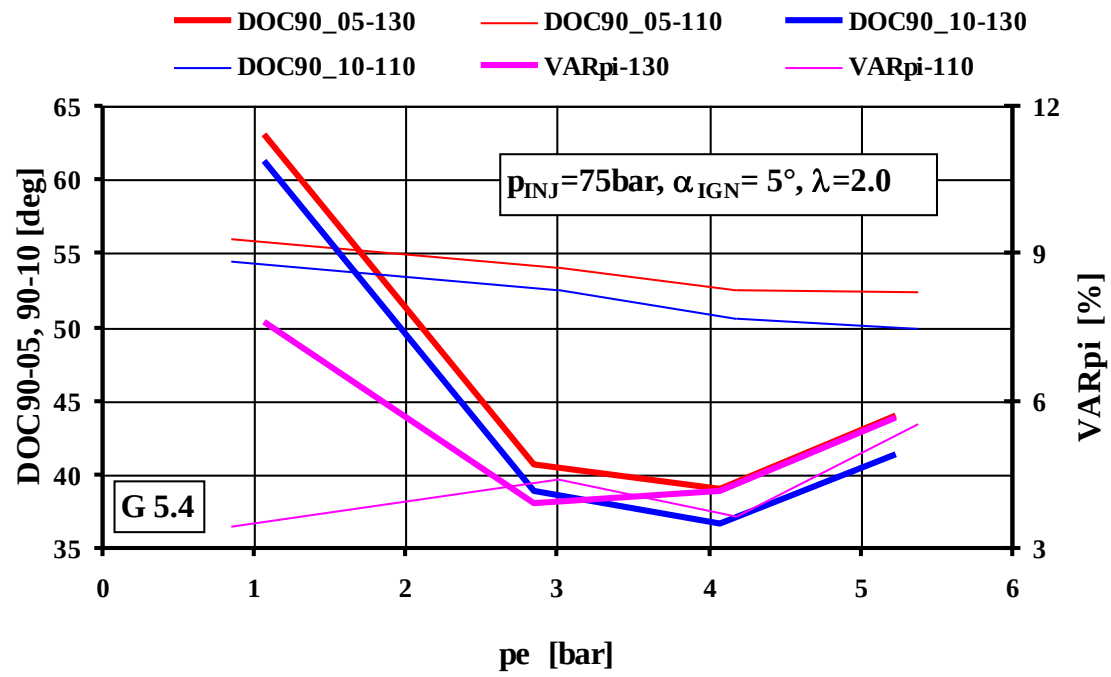


Figure G 4.1, G 4.2 and G4.5

The heat of combustion development versus rotational crank angle (degree) at 3000 1/min and various parameters (λ, p_{inj}, IGN and Inj) are plotted in Figure G 4.1 to 4.5.

The duration of heat release is prolonged with the increase of air excess ratio for the same p_{inj}, IGN and Inj. The reason can be attributed to low combustion temperature caused by lean combustion. The flame velocity is reduced with the decrease of combustion temperature, so that the flame development and propagation duration are both prolonged with the increase of air excess ratio.



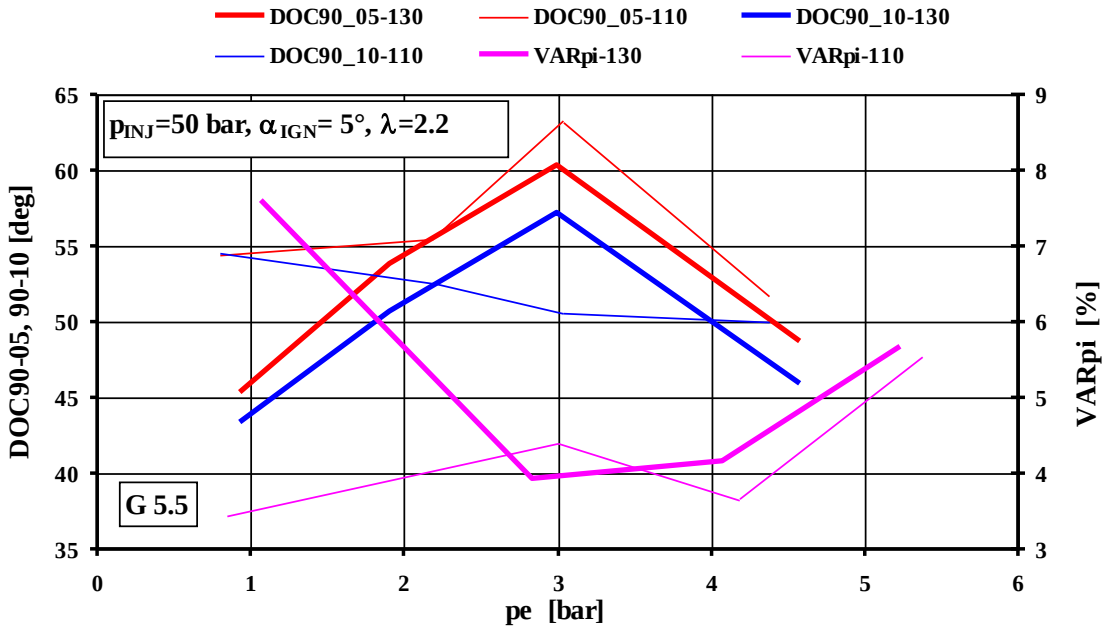
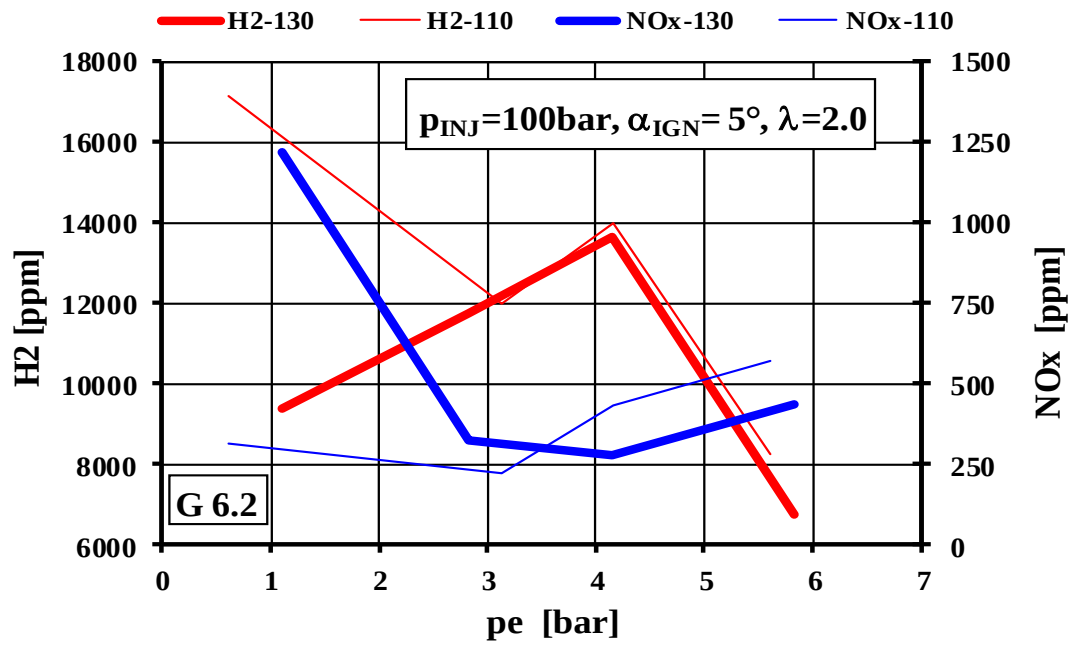


Figure G 5.4 and 5.5

Figure 5.4 and 5.5 show the phase of the combustion duration 5-90% and 10-90% at dependence on the mean effective pressure(pe) for two injection time (110 and 130°BTDC). In addition the duration of combustion, the graph is displayed on coefficient of variability in mean indicated pressure (VARpi). The fluctuation of VARpi shown in figure G 5.5 is small, however, it is enlarged in the figure 5.4. The maximum fluctuation takes place at low load of engine. The maximum burning duration at the middle of engine load for injection pressure of 50 bar occur while at low load for injection pressure of 75 bar. The plotted courses show the influence of the different timing of the fuel injection on the parameters of burning and on the variability of working cycle parameters – it is probably the relationship to inhomogenity of the mixture.



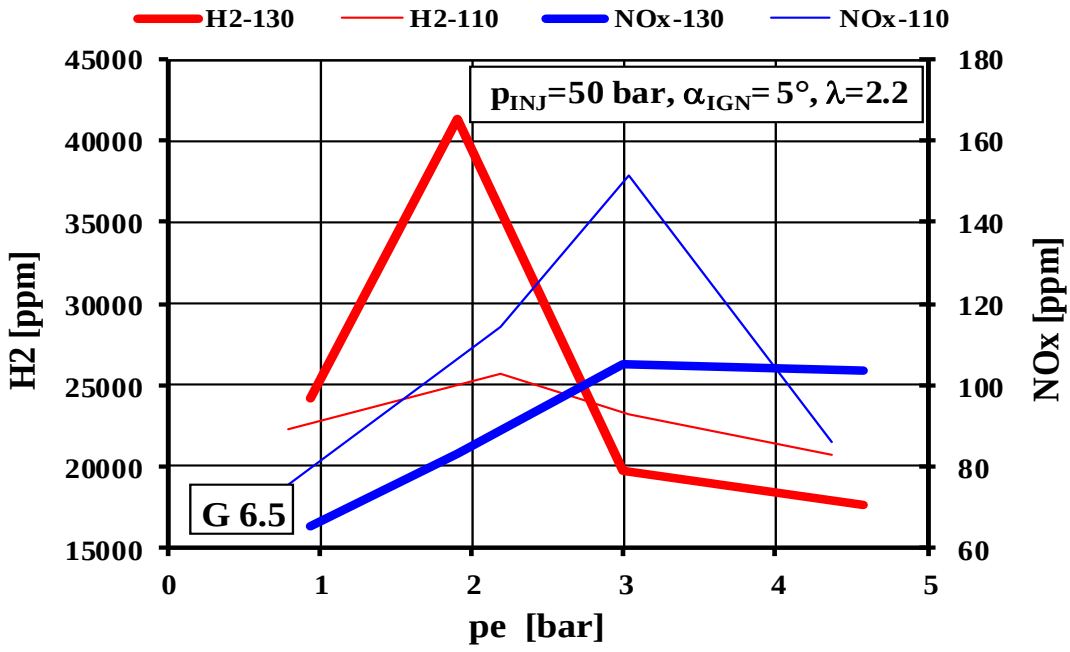


Figure G 6.2 and 6.5

The variation of NO_x and unburned hydrogen in emissions on mean effective pressure at 3000 rpm and different injection pressure and starting injection is demonstrated in figure 6.2 and 6.5. It is clearly seen that the maximum unburned hydrogen content was observed around the middle of load of engine with injection pressure of 100 bar and λ= 2.0 while at the low load of engine with injection pressure of 50 bar and λ= 2.2. NO_x emissions for injected pressure of 100 bar decrease with the increases of engine load (pe) while increase with increase of engine load compared with 50 bar of injection pressure. This demonstrated dependences they have again (probably) the consequence with the very short time for internal mixture forming and other relationship cannot be proof.

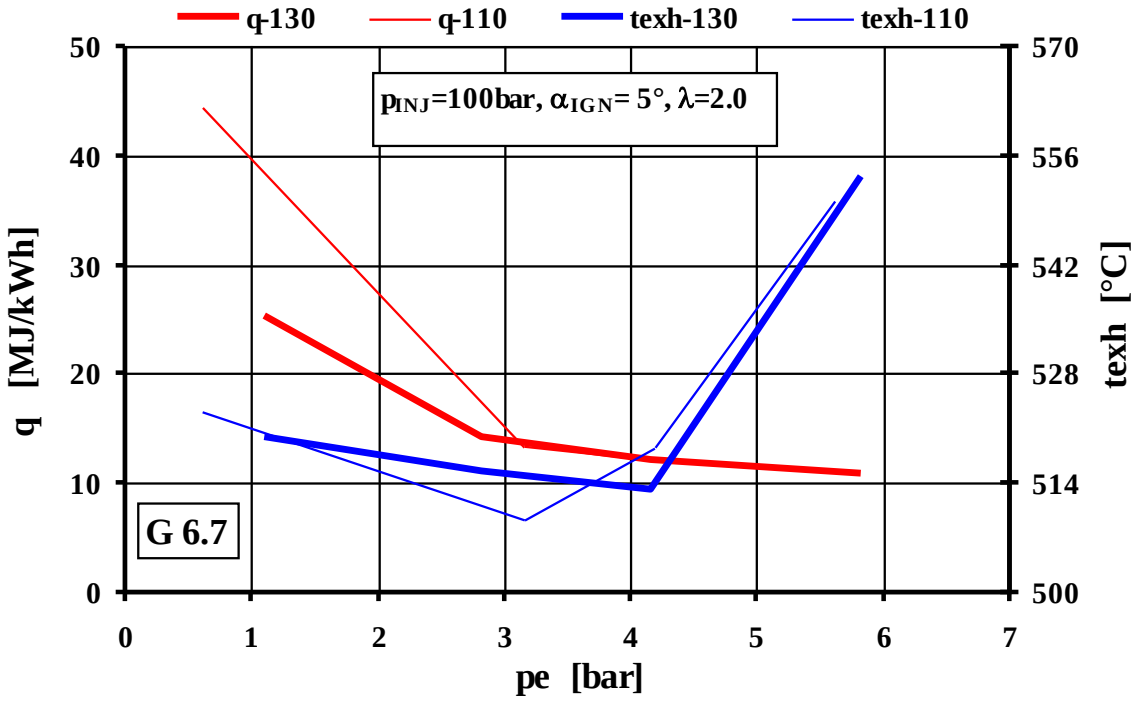
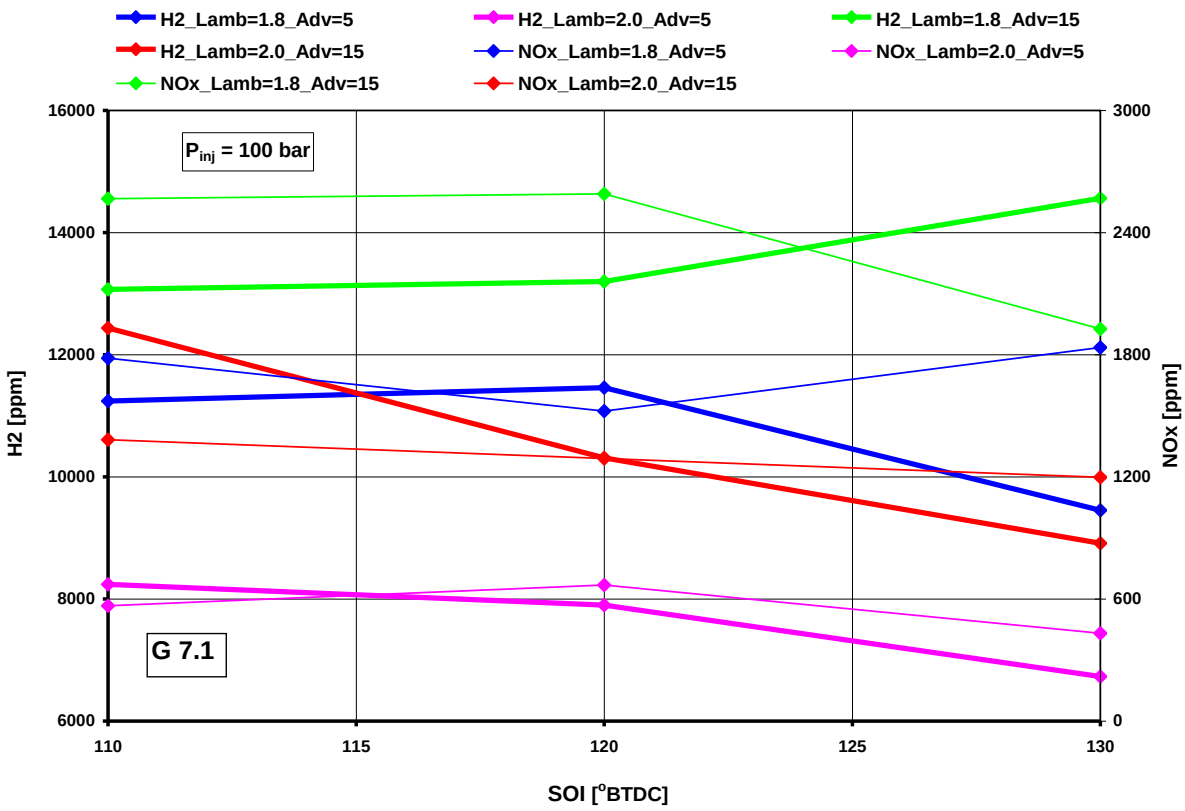


Figure G 6.7

Figure 6.7 shows the variation on heat of combustion (q) and exhaust gaseous temperature over mean indicated pressure (p_e) at 3000 rpm with different started injection of 110 and 130 ^{o}BTDC for selected injection pressure of 100 bar , air excess ratio of 2.0 and spark advance of 5 ^{o}BTDC. Generally, it is clearly to perceive from the figure that the decreases of heat by combustion with increases of engine loading, contrary, higher mean indicated pressure lead to increases of exhaust gas temperature. The fluctuation of injection time indicated in the range of low load is small. The effect of the injection time on the gas temperature in emission is not significant.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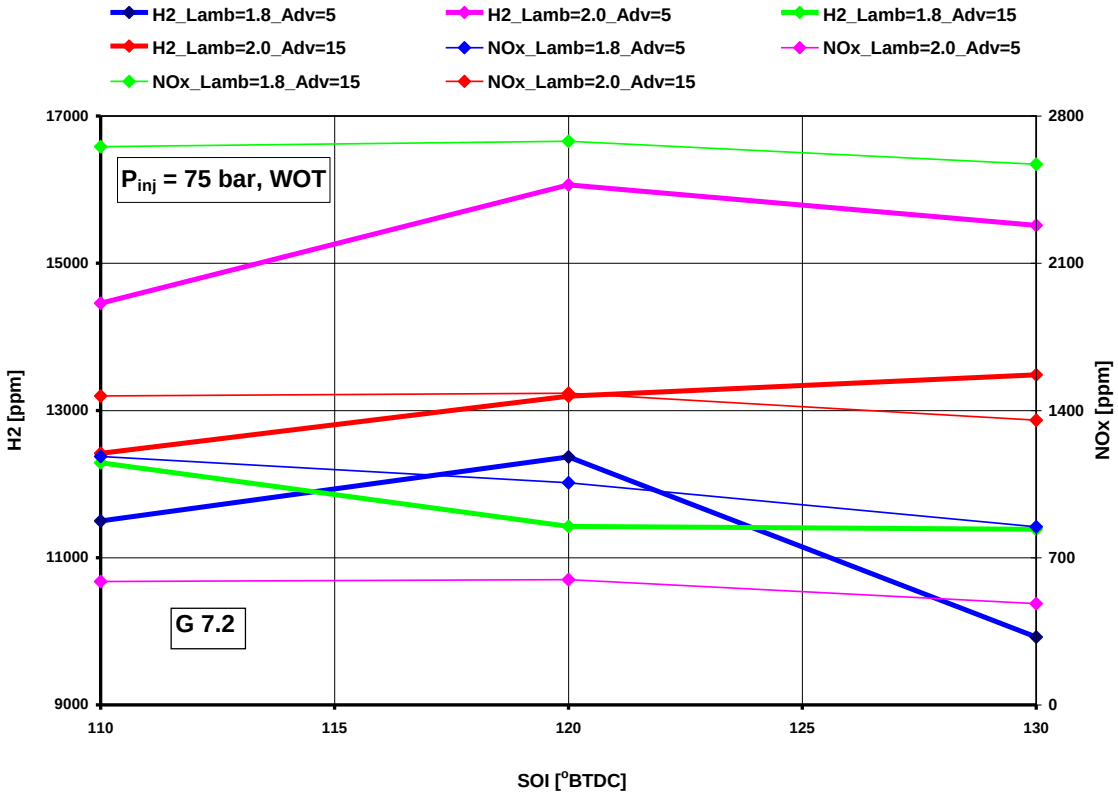
H2_Lamb=2.0_Adv=5
H2_Lamb=1.8_Adv=15
H2_Lamb=2.0_Adv=15
NOx_Lamb=1.8_Adv=5
NOx_Lamb=2.0_Adv=5
NOx_Lamb=1.8_Adv=15
NOx_Lamb=2.0_Adv=15
P_inj = 100 bar
G 7.1
H2 [ppm]
NOx [ppm]
SOI [°BTDC]
16000
14000
12000
10000
8000
6000
3000
2400
1800
1200
600
0
110
115
120
125
130


H2_Lamb=1.8_Adv=5
H2_Lamb=2.0_Adv=5
H2_Lamb=1.8_Adv=15
H2_Lamb=2.0_Adv=15
NOx_Lamb=1.8_Adv=5
NOx_Lamb=2.0_Adv=5
NOx_Lamb=1.8_Adv=15
NOx_Lamb=2.0_Adv=15
P_inj = 75 bar, WOT
G 7.2
H2 [ppm]
NOx [ppm]
SOI [°BTDC]
17000
15000
13000
11000
9000
2800
2100
1400
700
0
110
115
120
125
130

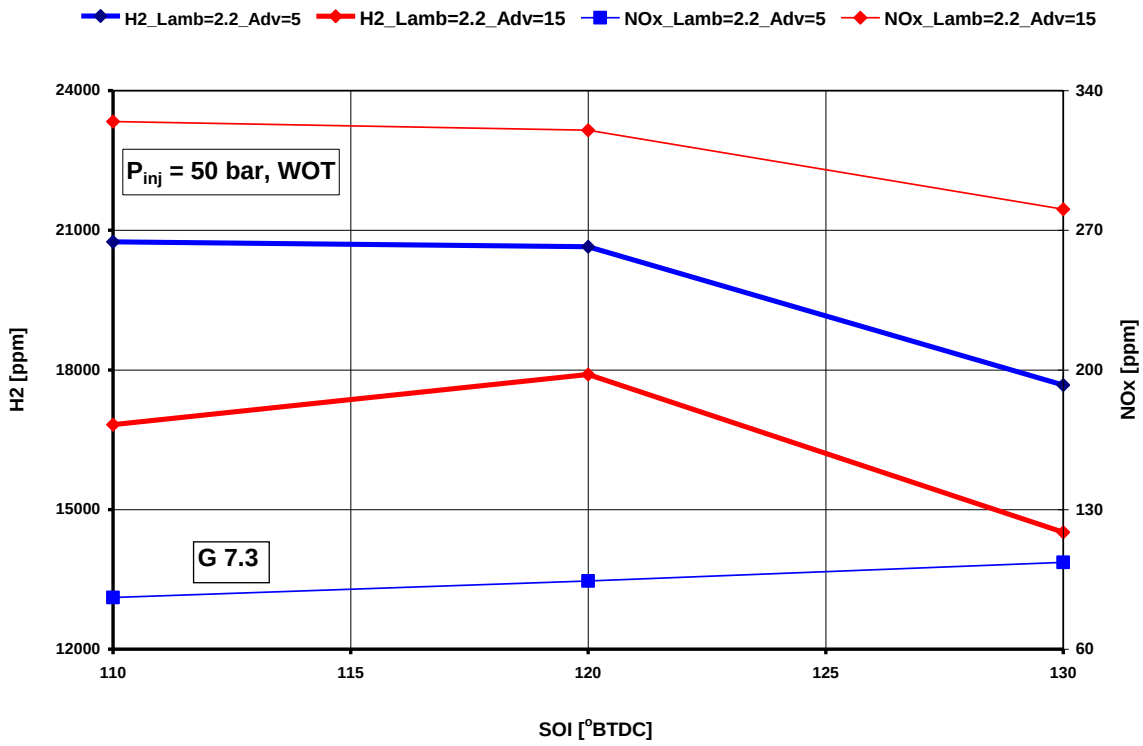
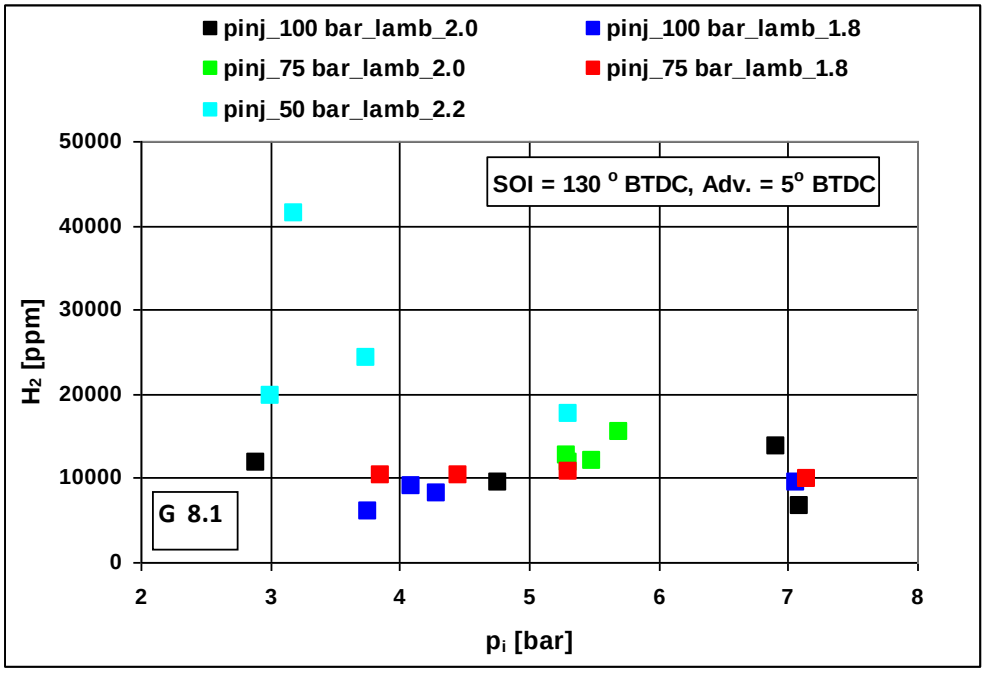


Figure G 7.1, 7.2 and 7.3

Figure 7.1, 7.2 and 7.3 display the variation of NO_x and unburned hydrogen level in emission with various starting injection at injection pressure of 100, 75 and 50 bar, respectively, for different air excess ratio(λ) and spark advance. The change of the NO_x concentration at exhaust gases on ignition advance has the standard character. Regarding to H_2 concentration (unburned) in exhaust gases has the certain dependence on the timing of fuel injection – the early start of injection leads to the lower value of H_2 concentration and it can be explain like the effect of the extension of the time for the preparation of the mixture.



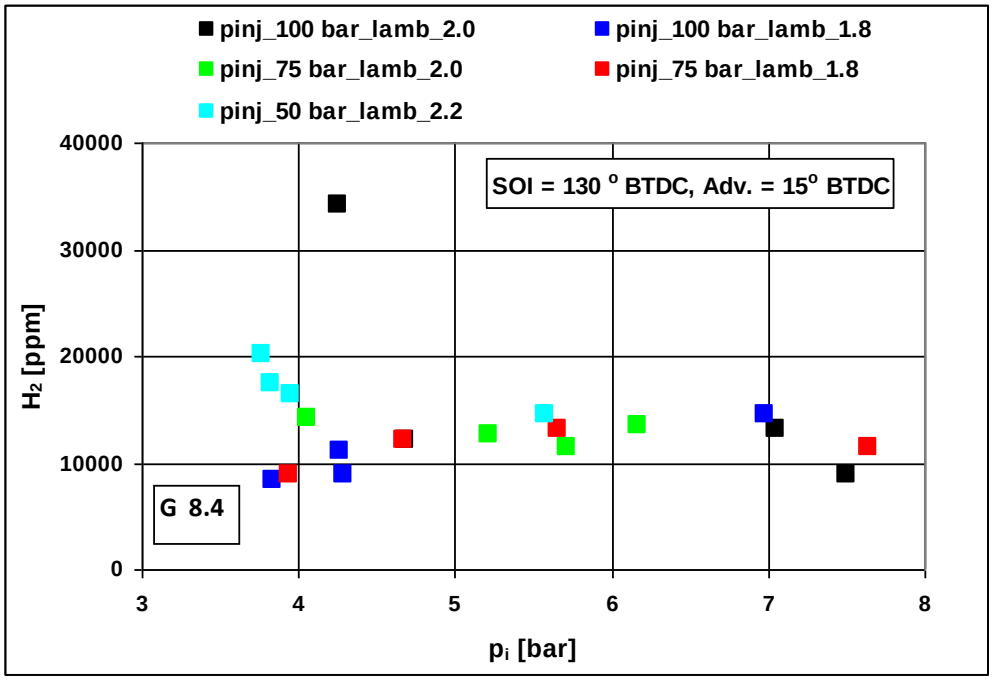
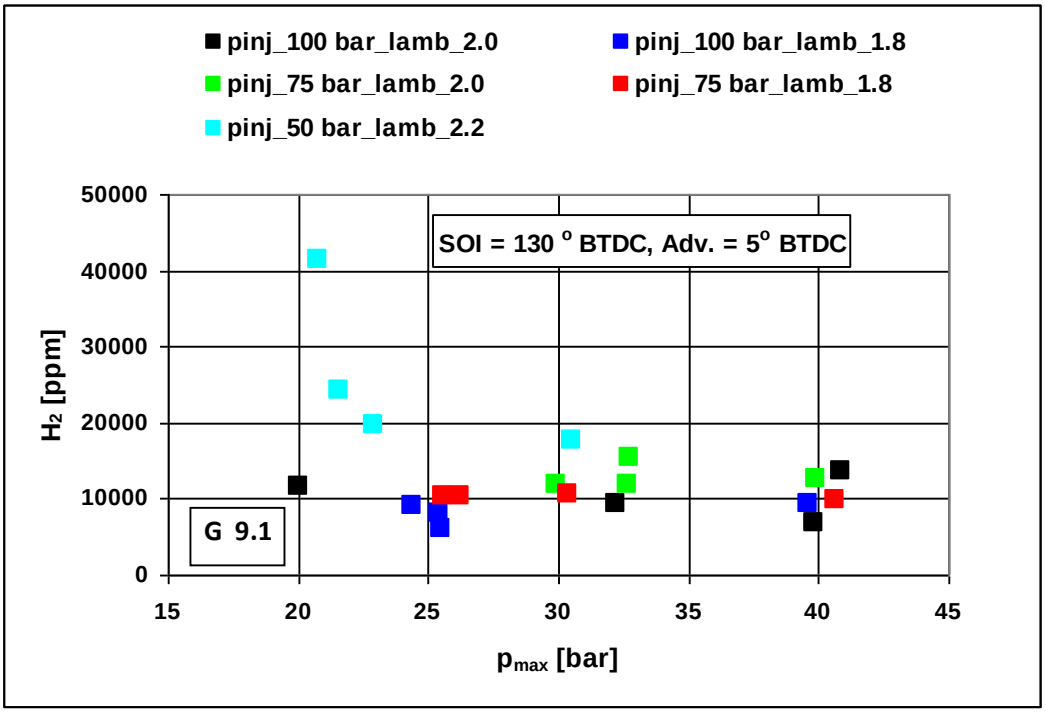


Figure G 8.1 and 8.4

Figure 8.1 and 8.4 show the relationship between mean indicated pressure (p_i) on unburned hydrogen level in emission at 3000 rpm with started injection of 130 ^{o}BTDC and different injection pressure, air excess ratio and spark advance. Generally, it is clearly to perceive from the figure that the fluctuation indicated in the figure is very small. The effect of the spark advance on the unburned hydrogen level in emission is not significant.



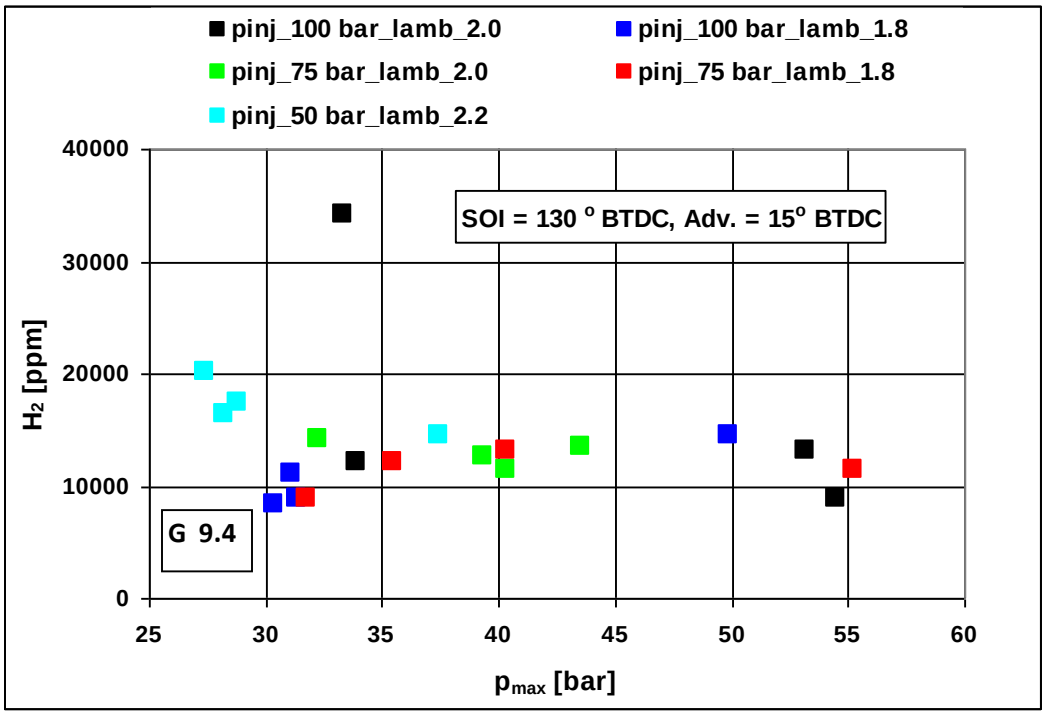
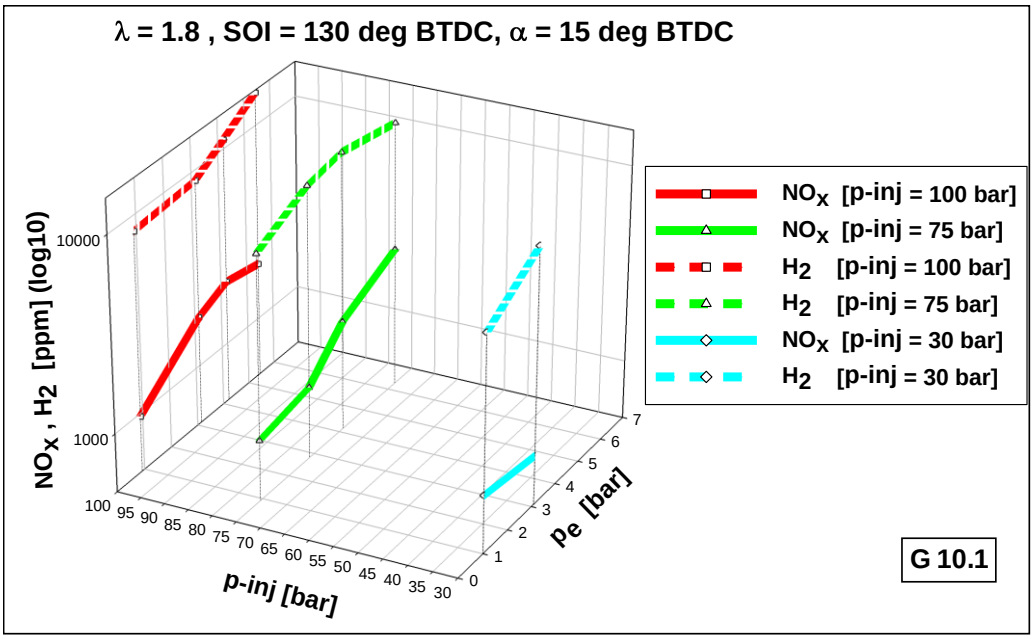


Figure G 9.1 and 9.4

The variation of unburned hydrogen content in exhaust gases with the maximum pressure in cylinder at 3000 rpm and starting injection of 130 °BTDC with various injection pressure and air excess ratio (λ). As it can be seen from figure 9.1 and 9.4, there are a significant fluctuation in unburned hydrogen level in emissions where the maximum pressure is low. Mostly, the level of unburned hydrogen in emission is quite steady, the relationship between unburned H_2 and p_{max} there is no.



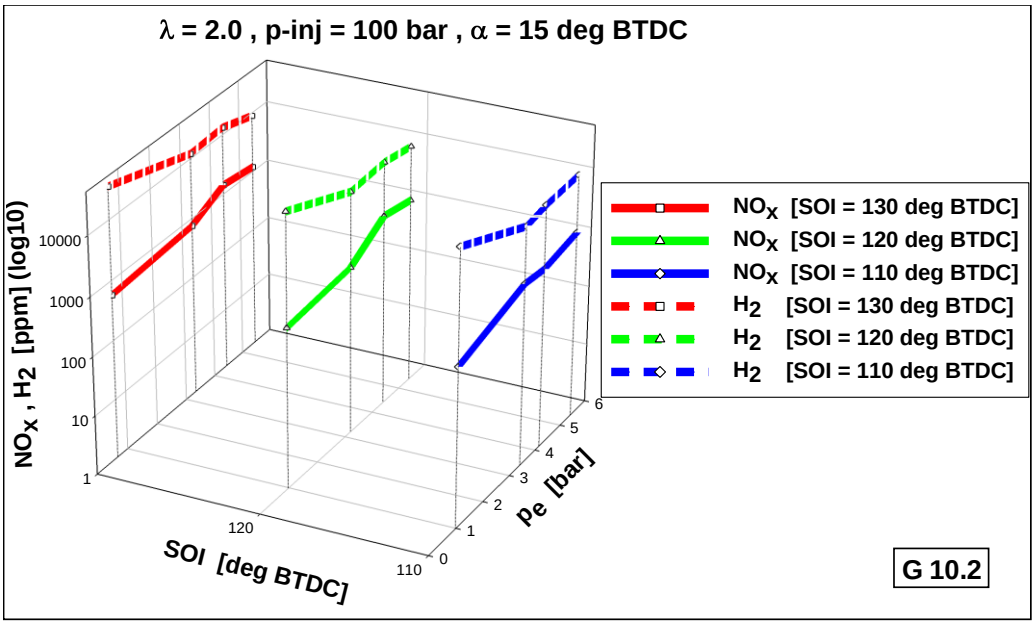


Figure G 10.1 and 10.2

Figure G 10.1 indicates the variation of NO_x concentration and unburned hydrogen with the changes of injection pressure and mean effective pressure for limited injection start (130° BTDC), lambda of 1.8 and ignition start of 15° BTDC. It can be observed that the increases of unburned hydrogen level and NO_x concentration with increases of mean indicated pressure at each constant of injection pressure. Figure G 10.2 describes that the minimum of unburned hydrogen takes place around middle of mean indicated pressure at each fixed start of injection. It is clearly seen that NO_x level go up with increases of mean indicated pressure. For hydrogen engine, very high concentration of hydrogen in exhaust gases depends on injection pressure, start of injection and loading of engine (p_e).

The relatively high concentration of the unburned hydrogen in exhaust gas was surprising results. Experimental engine has unacceptable fall of parameter burning mixtures and content of unburned fuel in exhaust gases. The verification of single systems of engine found out no function failure, the reason was consequently predicated to the great inhomogeneity of the mixture by the effect of very short time for mixture forming in cylinder motor during compression stroke. Therefore there was fulfillment comparison of results measurement on experimental engine at running on CNG with the direct of high pressure injection CNG (DI = 100 bar, with the identical timing of the injection like for hydrogen) with the measurement on identical (but unmodified, original) engine type at running on CNG with the low-pressure injection of CNG to the engine inlet manifold (MPI).

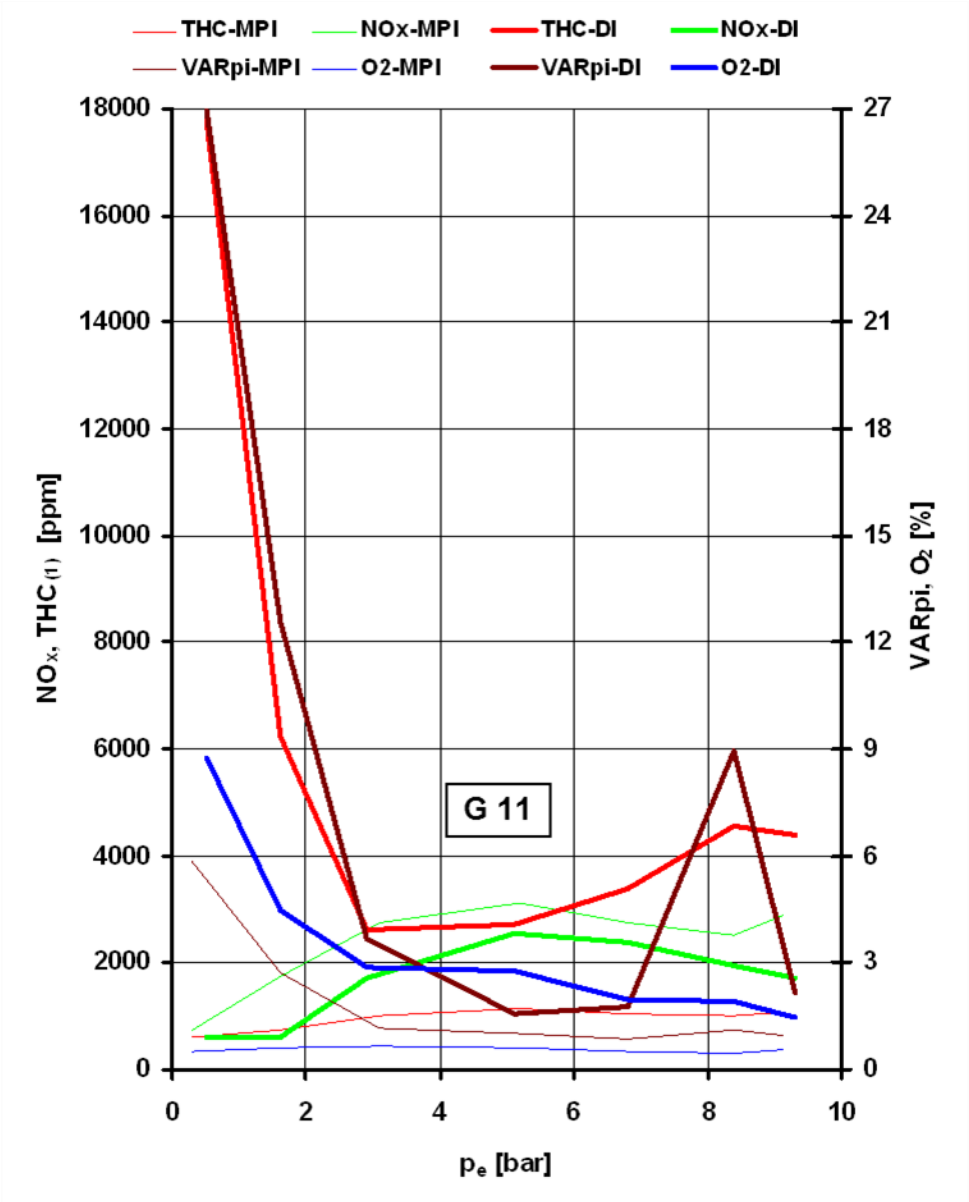


Figure G11: Comparison of the selected parameters of the SI experimental hydrogen engine (DI) and the same type (original) engine MPI for running on CNG. Both engines were operated on n=3000 rpm and λ=1. The incomplete combustion of mixture for DI engine there is demonstrated by the higher concentration of unburned $THC_{(1)}$ and residual oxygen O_2 in exhaust gases also.

The results of the comparison are showed at graph. Practically, all range of operating condition, the DI engine produces higher concentration of unburned H_2 in exhaust gases. It also indicates the greater inhomogeneity of mixtures for DI engine. The fundamental course of mixture burning leads to high cycle to cycle variability and also reduces efficiency of engine.

The experimental program on gas fueled experimental engine with internal mixture formation using high-pressure injection of gaseous fuel to the engine cylinder shows a possibility of technical realization of high-speed vehicle gas-engine with direct injection of gaseous fuel to the cylinder engine. The technical solution of engine has the great signification for using hydrogen like fuel for internal combustion engine. The obstacles have been shown by the results of performed measurements that require technically solution. The improvement of mixture homogeneity might be solved by suitable directions of gaseous fuel spray from injector, adjustment of combustion-chamber shape, increasing the swirl in cylinder engine, etc. For optimizing of internal mixture mechanism formation must use the simulation model of internal aerodynamics in cylinder, CFD approach.

The high content of hydrogen in the exhaust gas could be also by incidence of the leakage at high pressure injector. Because the experimental program on the experimental engine must have been untimely ended for sudden effect of the big leakage in injector, it has not been possible to realize further testing program on experimental engine (e.g. the different directions of the hydrogen outflow from the injector to the cylinder charge).

CHAPTER 6

COMPUTATIONAL ESTIMATION OF THE POWER AND EMISSION PARAMETERS OF THE HYDROGEN ENGINE

The performed experiment demonstrate, at harmony to cited property of hydrogen like engine fuel, that the hydrogen piston engine there is possible to operate safely without knocking if the engine running to very poor mixture. Be evidenced, that at mean speed regime of the natural aspirated engine on $\lambda = 1.8$ and 100% load (WOT) there is combustion process without knocking both at ignition advance 5 °BTDC ("standard" ignition advance), position $p_{max} \cong 15$ °ATDC), so at increasing of ignition advance to 15°BTDC (position $p_{max} \cong 5\text{-}10$ °ATDC).

The power characteristics of the natural aspirated of the hydrogen experimental engine at combustion of hydrogen-air mixture with $\lambda = 1.8$ they are however relatively low at comparison to standard parameters of SI engine for running on petrol ($\lambda \cong 1$). For the reaching of hydrogen engine power parameters, that have will a comparable to power properties of the original SI engine at his running on petrol, must be using the concept of the supercharged engine with the combustion of very poor mixture.

By means of computational program "Tlak.xls" [44] that was performed the computational estimation of the power and emission behavior of the experimental hydrogen engine for natural aspirated and supercharged engine version. Characteristics course burning was determined according to course combustion speed (ROHR) of hydrogen-air mixtures, that have was evaluated by the thermodynamic analyses of the measured pressure course in cylinder engine (graphs G3 in Appendix 1): the total burning time has been estimated according to period of the main combustion process (without phase afterburning). The method of the calculation NO production in the cylinder engine it is explain more detail at Appendix 2. The results of these calculations they show the graphic elaboration at figure 12.2. At graph there are showed for the comparison the measured parameters of the original SI engine at running on petrol. The singles variants of engines at graphs they are:

1. The original vehicle SI engine at running on petrol (WOT) with the control of the richness mixtures and ignition advance by original ECU.
2. The experimental SI natural aspirated engine at running on hydrogen at 100% load regime (WOT) with the richness mixture $\lambda = 1.8$ and ignition advance 5 °BTDC.
3. The experimental SI supercharged engine at running on hydrogen at 100% load regime (WOT) with the richness mixture $\lambda = 2.2$ and ignition advance 5 °BTDC. The boost pressure of air there was determined so as to power parameters of the engine there was near to original engine at running on petrol.

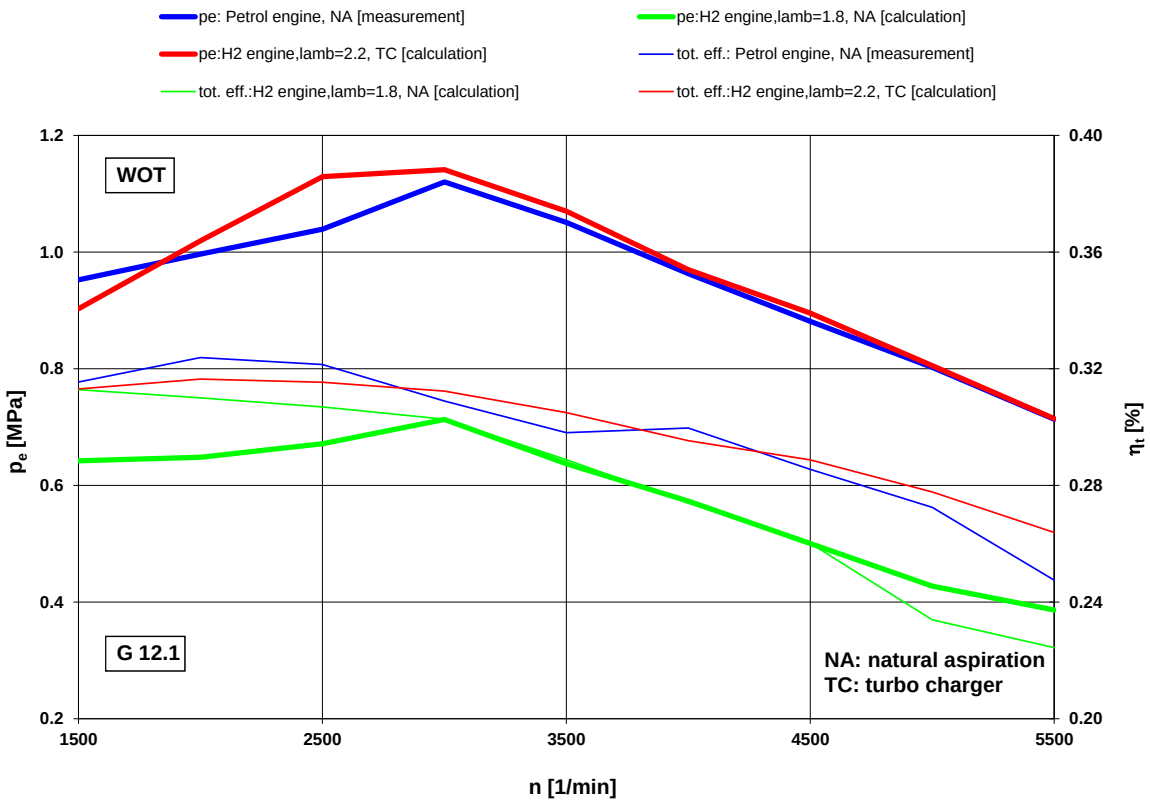


Figure G 12.1

The graph displays total efficiency (η_t) and means indicated pressure (p_i) versus engine speed at fully wide throttle, spark advance of 5 °BTDC and air fuel ratio of 1.8 and 2.2 for three different type of engine which are calculation and measurement.

As can be seen from the figure, the maximum efficiency for all engines occurs near the middle speed of around 3000 1/min. The hydrogen fuelled engine with turbocharger and the naturally aspirated petrol engine can produce higher mean indicated pressure and efficiency compared to the other hydrogen fuelled engine without turbocharger over all range of engine speed. Moreover, two first engines have similar performance.

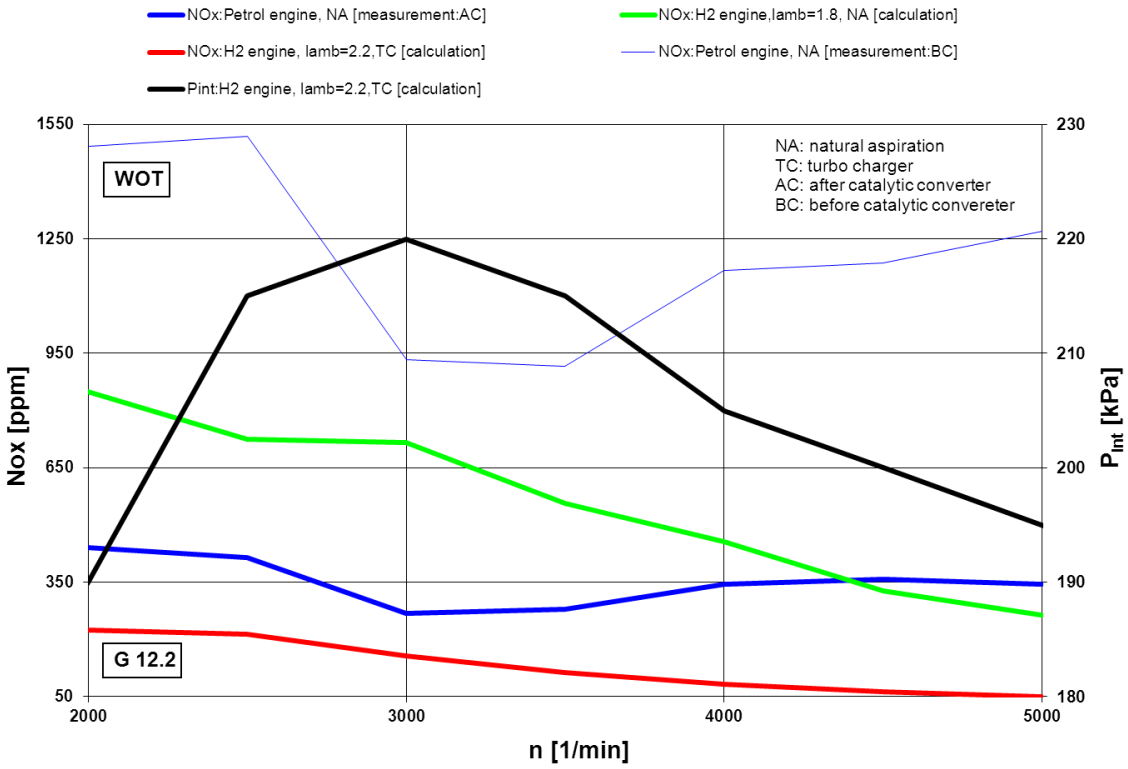


Figure G12.2

The variation of NO_x level in emissions with engine speed at full load (WOT) for different air fuel ratio of 1.8 and 2.2 and spark advance of 5 ^{o}BTDC is demonstrated in figure G12.2.

It is clearly seen that the maximum NO_x content was observed at low speed of engine. In general, it is obtained from the results that the decreases of NO_x emission with increases of engine speed. The hydrogen fuelled engine with turbocharger limited air fuel ratio (λ) of 2.2 can release the minimum NO_x content compared to the same engine without turbocharger controlled λ of 1.8 that emits the highest level of NO_x.

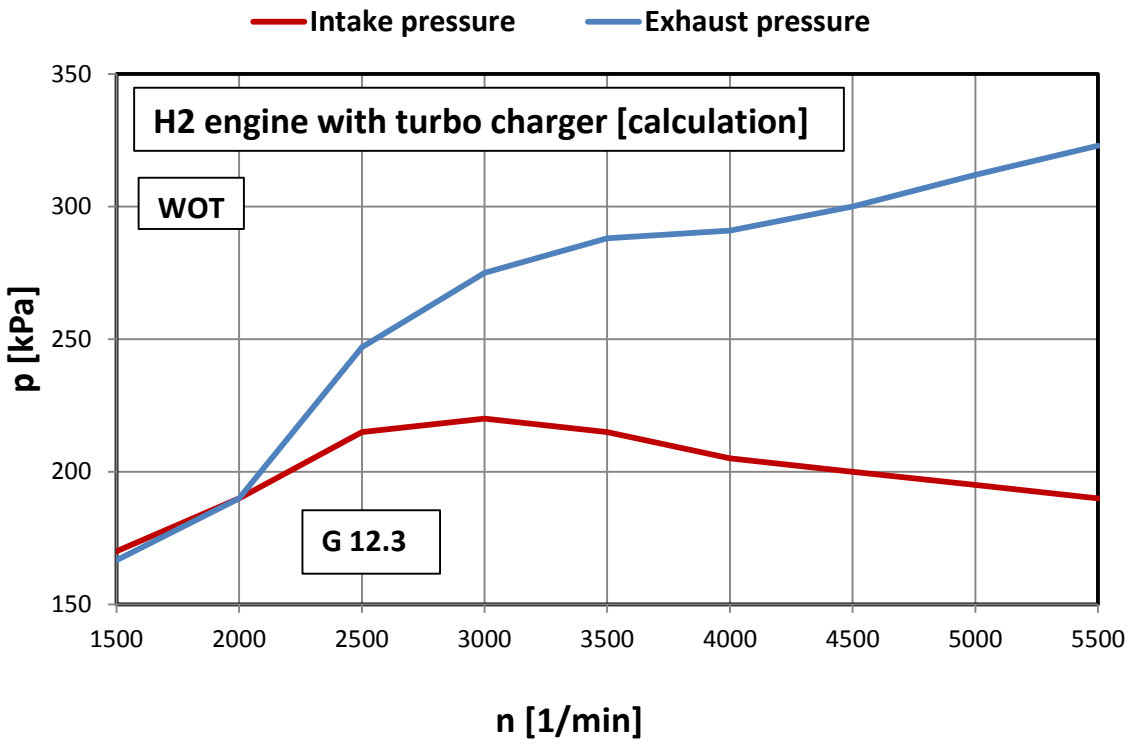


Figure G12.3

The courses of the mean values of the intake air pressure (in inlet manifold) and the exhaust pressure at the outlet from the exhaust port of engine for the turbocharged hydrogen engine for the set-up with the very lean mixture ($\lambda = 2.2$). The values of the intake pressure they were determined by the computational estimation for the fulfillment of the very near power parameters of the hydrogen engine like original petrol engine. The values of the exhaust pressure they are determined by the estimation using of the measured values of the exhaust pressure on the similar turbocharged engine (petrol engine, stoichiometric mixture, for power parameters higher upon 50% to original naturally aspirated petrol engine).

CONCLUSION

The study, experimental and computational parts of the thesis reflect, that the hydrogen is very first-rate engine fuel. For practical utilization of hydrogen in vehicle engine must be solved the safety, structural and motor management problems, which are determined by specific characteristics of hydrogen.

The internal mixture forming it is for hydrogen piston engine a very suitable solution. With reference to substances properties of hydrogen (especially to low density) there must be for internal mixture forming at course of compression stroke of piston the using of high pressure injection (insufflations) of gaseous hydrogen. The very short time for mixture forming in cylinder there requires the solving of the mixing flow of hydrogen with air cylinder charge (both experimentally the directions of outflow hydrogen from the injector and by means of CFD simulation).

The specific property of hydrogen is also the big ability of its penetration through the extremely small cross-section. For every piston engine they are such cross-section the piston rings. In light of the safety of hydrogen engine running is as well necessary to watch the hydrogen concentration in the crankcase of engine and by effective crankcase ventilation to the suction manifold of engine there must be remove the possible hazard state.

The contribution of this thesis for investigation of hydrogen engine they are at experimental research of the hydrogen engine properties with the direct high pressure injection of gaseous hydrogen to the engine cylinder during compression stroke. The results of the dissertation work reflect the basic characteristics of burning course of hydrogen-air mixture in cylinder, the characteristics of working engine cycle and emission engine data on dependence to engine adjustment (richness mixtures, ignition advance). The dissertation work as well shows on problems that are linked to internal mixture formation.

ABSTRAKT

Disertační práce se věnuje vodíku jako palivu pro pístový spalovací motor a připomíná vodík jako obnovitelný zdroje energie a minimální environmentální důsledky při spalování vodíku. V úvodních kapitolách jsou vysvětleny vlastnosti vodíku (pozitivní i negativní) a možné způsoby jeho výroby. Kapitoly rovněž ukazují dosavadních poznatky, zkušenosti a vlastnosti realizovaných vodíkových motorů a ukazují možnosti uložení vodíku v nádržích vozidla.

Hlavní částí disertační práce je experimentální laboratorní výzkum na tříválcovém vodíkovém motoru s tvořením směsi přímým vysokotlakým vstřikem plynného vodíku do válců motoru. Vodíkový motor vznikl konverzí původního zážehového motoru ŠA 1.2 HTP (EA111.03D) v laboratoři Katedry vozidel a motorů na Fakultě strojní Technické univerzity v Liberci. Pro ovládání a regulaci palivového systému (Common Rail), regulaci bohatosti směsi a předstihu zážehu vodíkového motoru a monitoring provozních parametrů motoru byla vytvořena speciální elektronická řídící jednotka.

Výzkumný program na vodíkovém motoru byl zaměřen na studium pracovního oběhu a vlastností motoru v závislosti na časování vstřiku a vstřikovacím tlaku vodíku, na bohatosti směsi, na zatížení motoru a na předstihu zážehu. Při všech měřeních byla prováděna vysokotlaká indikace s termodynamickou analýzou a statistickým zpracováním parametrů pracovního oběhu. Měřena byla i koncentrace NO_x a nespáleného H_2 ve výfukových plynech. Data ze všech měření byla archivována systémem automatizovaného sběru dat.

Výsledky provedených měření byly zpracovány graficky a jsou komentovány v samostatné kapitole. Velkým problémem u současného provedení experimentálního vodíkového motoru je vysoká koncentrace nespáleného H_2 ve výfukových plynech. Disertační práce ukazuje, že tento problém souvisí s použitým způsobem vnitřního tvoření směsi a doporučuje potřebná řešení k odstranění zjištěného problému.

Poslední kapitola obsahuje výsledky výpočtového řešení výkonových a emisních vlastností vozidlového vodíkového motoru pro dvě různá seřízení a porovnává tyto výsledky s vlastnosti původního motoru při provozu na benzin.

ABSTRACT

The dissertation work deals with the hydrogen as a fuel for internal combustion engines and hydrogen points as renewable energy and minimal environmental consequences of burning hydrogen. The first chapter introduces and explains the properties of hydrogen both positive and negative side, and possible ways of its production. It also present piece of knowledge, experiences and properties of the realized hydrogen engine and reflect the possibilities for the storage of hydrogen in the vehicles tanks.

The main part of the dissertation work is the experimental laboratory research on three cylinder hydrogen SI engine with the forming of mixtures by the direct high pressure injection of the gaseous hydrogen to the cylinder engine. The experimental hydrogen engine has been conducted by conversion of the original SI engine Škoda Auto 1.2 HTP (EA111.03D) at the Department laboratory of vehicles and engine on Faculty of mechanical engineering on Technical University of Liberec. The special electronic control unit was programed and implemented for the control and regulation of the fuel system (Common Rail), regulation of richness mixtures and ignition advance as well monitoring of the operational hydrogen engine data also.

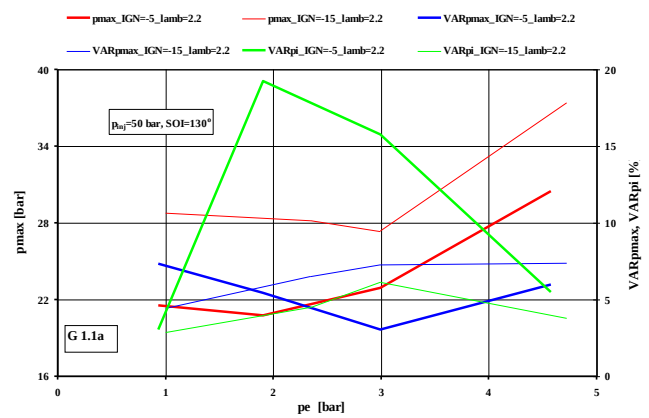
The experimental research program on hydrogen engine was orientated to research of the working cycle and engine behavior that are depend on injection timing and injection pressure of hydrogen with various on richness mixtures, load of engine and ignition advance. All measurements were performed with a high indication of thermodynamic analysis and statistical processing of working cycle parameters. The concentration of NO_x and unburned H_2 in exhaust gas has been measured also. The data from of all metering has been archived by the system of automated data collection.

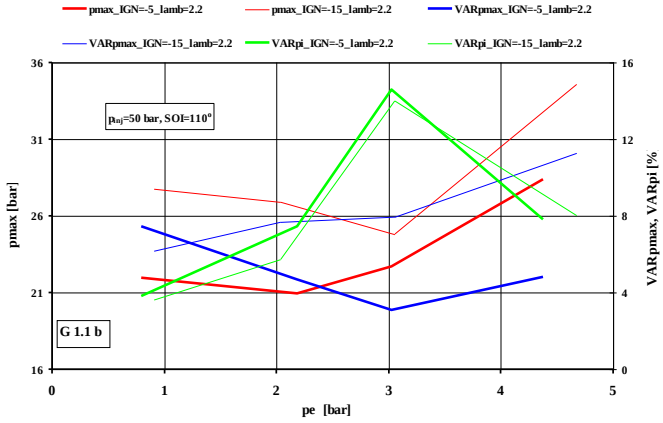
The results of the measurements were processed graphically and their relationships were described in a separate chapter. The big problem of the contemporary design of the experimental hydrogen engine is the high concentration of unburned H_2 in exhaust gas. The dissertation work shows that this problem be connected with the applied technique for the inner mixture formation and recommend the needed solution for the elimination of the recognized problem.

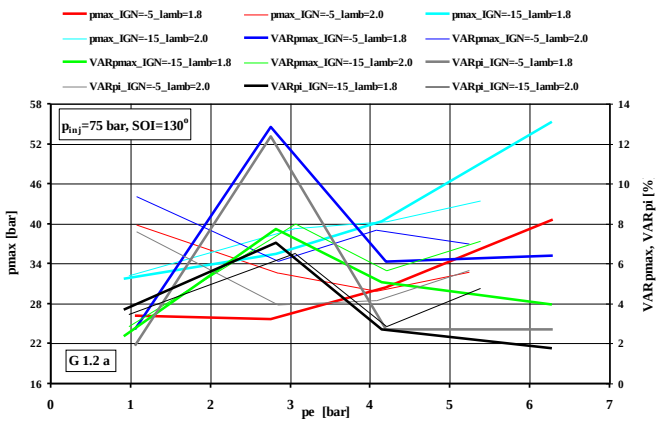
The last chapter contains the results of the computational solution of the power and emission behaviors of the hydrogen vehicle engine for two different setting of the hydrogen engines and these results are compared to properties of the original engine at running on petrol.

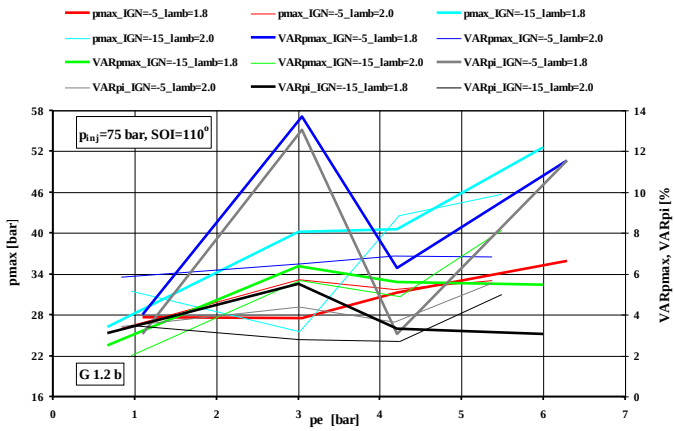
APPENDIX 1

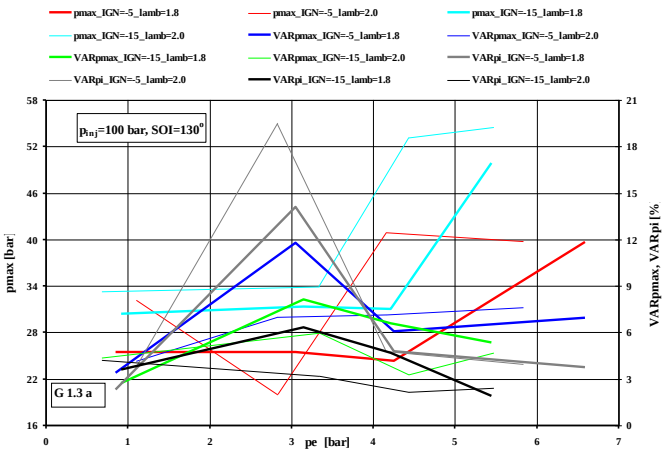
The graphs of experimental hydrogen fuelled engine.

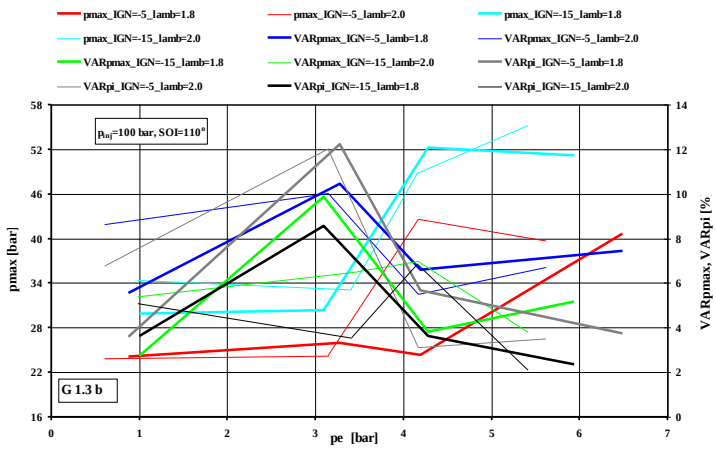


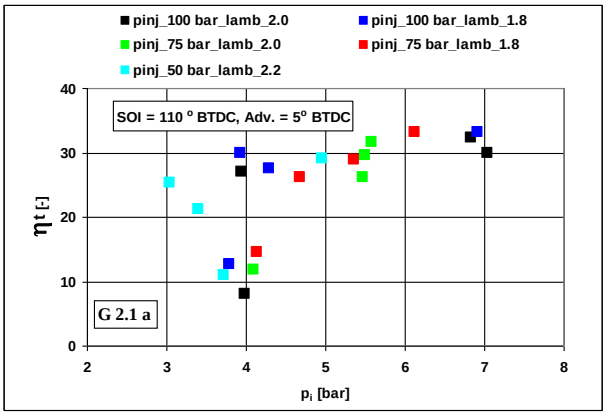








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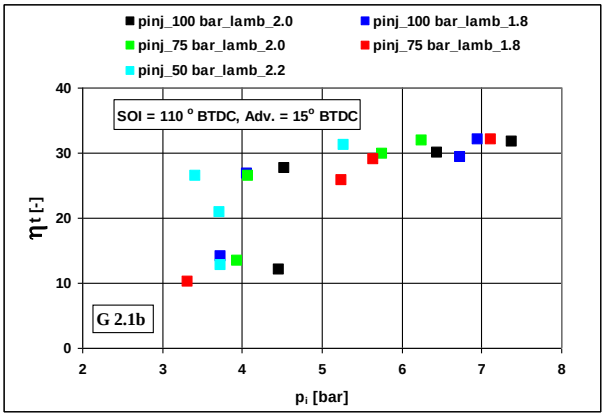
pinj_100 bar_lamb_1.8
pinj_75 bar_lamb_2.0
pinj_75 bar_lamb_1.8
pinj_50 bar_lamb_2.2
SOI = 110 ° BTDC, Adv. = 5° BTDC
G 2.1 a
ηt [-]
pi [bar]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pinj_100 bar_lamb_1.8
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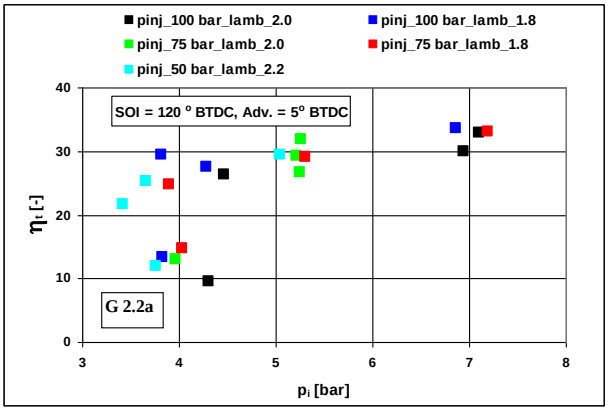
pinj_75 bar_lamb_1.8
pinj_50 bar_lamb_2.2
SOI = 110 ° BTDC, Adv. = 15° BTDC
G 2.1b
ηt [-]
pi [bar]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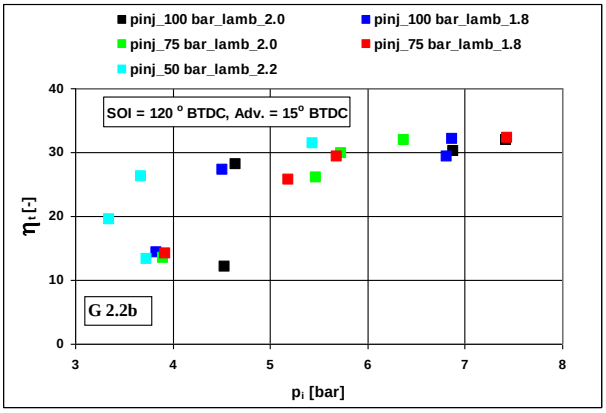
pinj_100 bar_lamb_1.8
pinj_75 bar_lamb_2.0
pinj_75 bar_lamb_1.8
pinj_50 bar_lamb_2.2
SOI = 120 ° BTDC, Adv. = 5° BTDC
G 2.2a
ηt [-]
pi [bar]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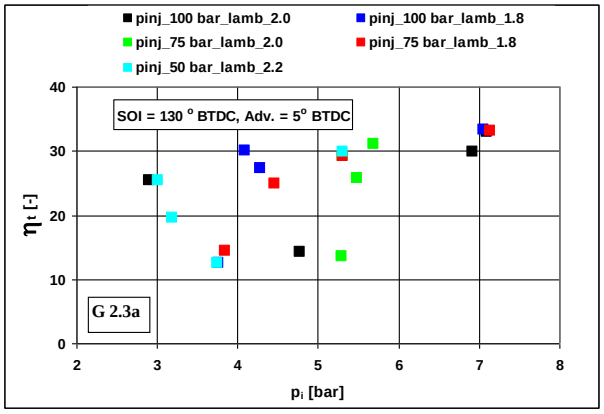
pinj_75 bar_lamb_1.8
pinj_50 bar_lamb_2.2
SOI = 120 ° BTDC, Adv. = 15° BTDC
G 2.2b
ηt [-]
pi [bar]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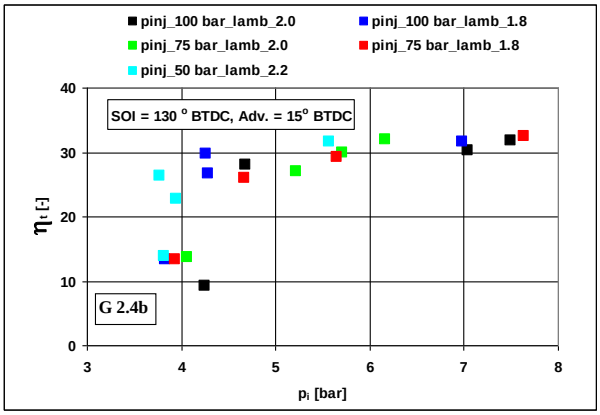
pinj_75 bar_lamb_2.0
pinj_75 bar_lamb_1.8
pinj_50 bar_lamb_2.2
SOI = 130 ° BTDC, Adv. = 5° BTDC
G 2.3a
ηt [-]
pi [bar]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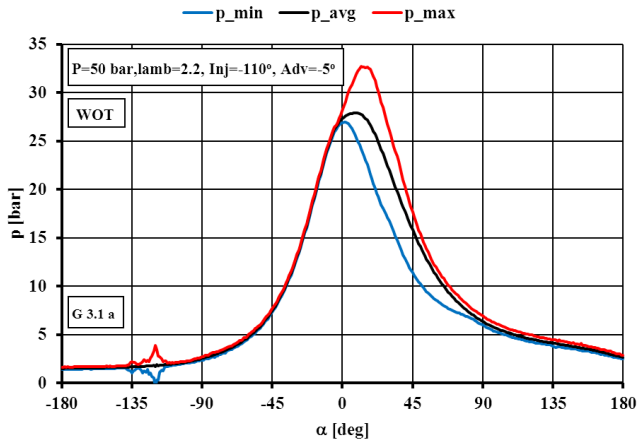
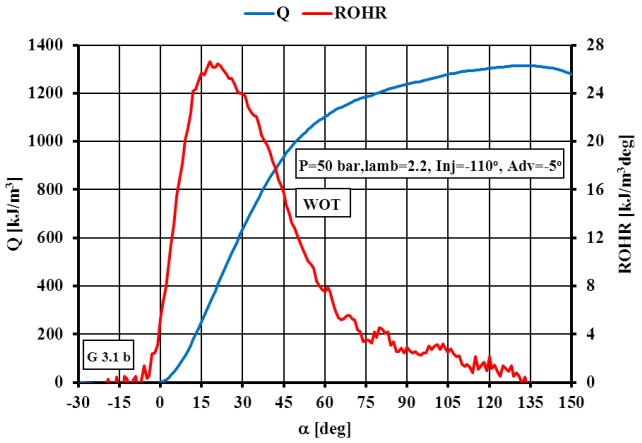
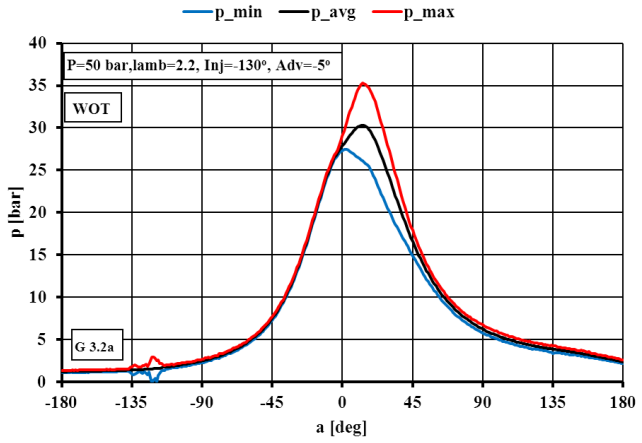
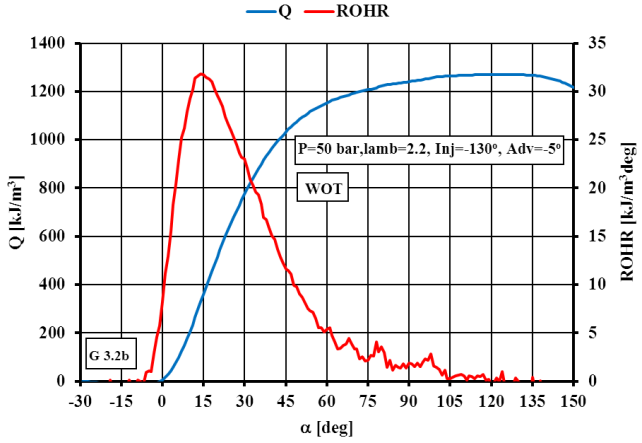
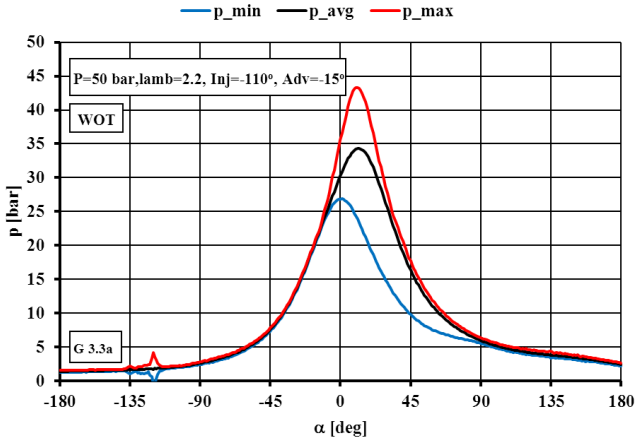
pinj_100 bar_lamb_1.8
pinj_75 bar_lamb_2.0
pinj_75 bar_lamb_1.8
pinj_50 bar_lamb_2.2
SOI = 130 ° BTDC, Adv. = 15° BTDC
G 2.4b
ηt [-]
pi [bar]

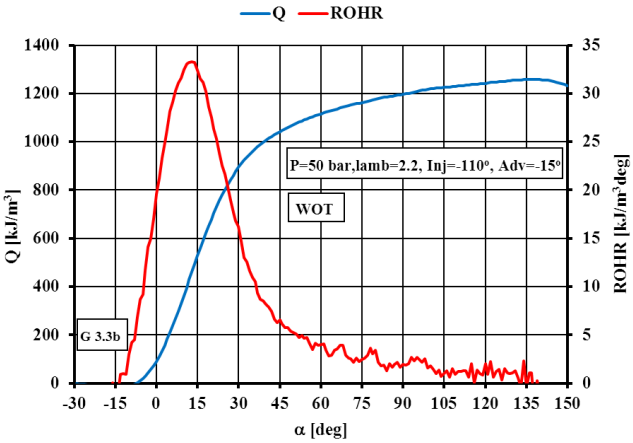

p_min
p_avg
p_max
P=50 bar,lamb=2.2, Inj=-110°, Adv=-5°
WOT
G 3.1 a
p [bar]
α [deg]

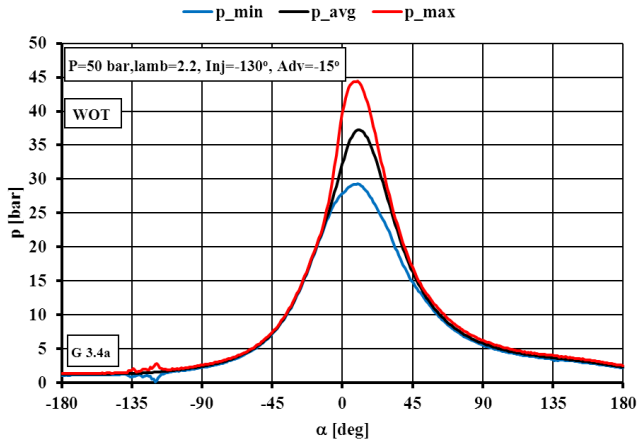

Q
ROHR
P=50 bar,lamb=2.2, Inj=-110°, Adv=-5°
WOT
G 3.1 b
Q [kJ/m³]
ROHR [kJ/m³deg]
α [deg]

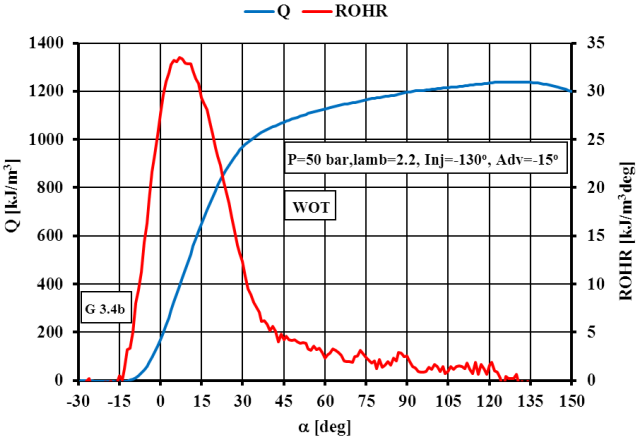

p_min
p_avg
p_max
P=50 bar,lamb=2.2, Inj=-130°, Adv=-5°
WOT
G 3.2a
p [bar]
a [deg]

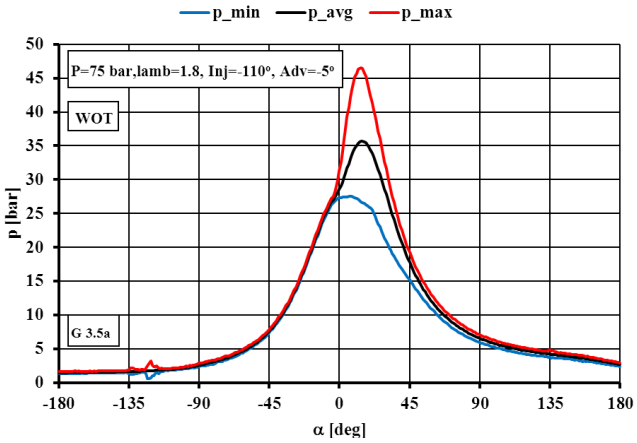

Q
ROHR
P=50 bar,lamb=2.2, Inj=-130°, Adv=-5°
WOT
G 3.2b
Q [kJ/m³]
ROHR [kJ/m³deg]
α [deg]

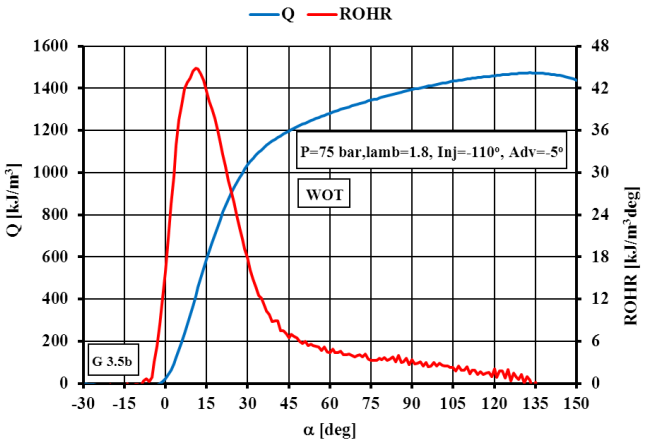

p_min
p_avg
p_max
P=50 bar,lamb=2.2, Inj=-110°, Adv=-15°
WOT
G 3.3a
p [bar]
α [deg]

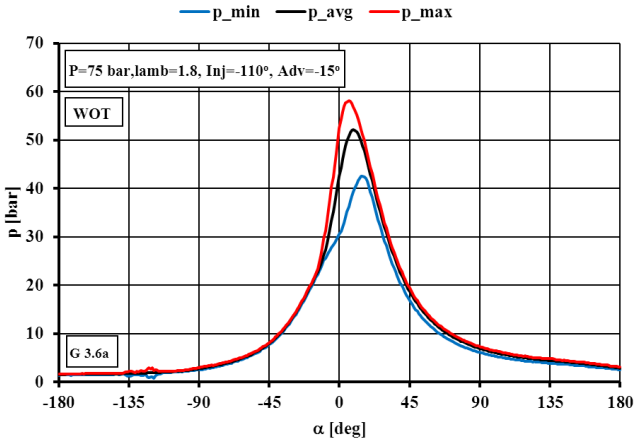

Q
ROHR
P=50 bar,lamb=2.2, Inj=-110°, Adv=-15°
WOT
G 3.3b
Q [kJ/m³]
ROHR [kJ/m³deg]
α [deg]

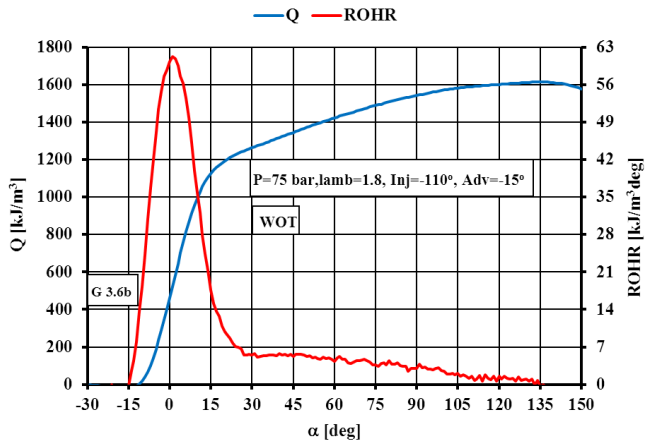

p_min
p_avg
p_max
P=50 bar,lamb=2.2, Inj=-130°, Adv=-15°
WOT
G 3.4a
p [bar]
α [deg]

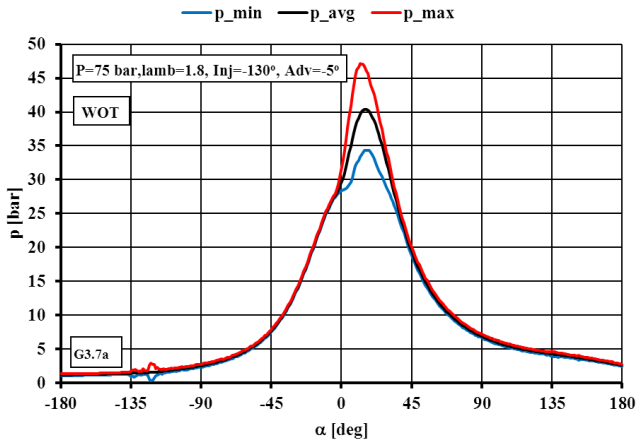

Q
ROHR
P=50 bar,lamb=2.2, Inj=-130°, Adv=-15°
WOT
G 3.4b
Q [kJ/m³]
ROHR [kJ/m³deg]
α [deg]

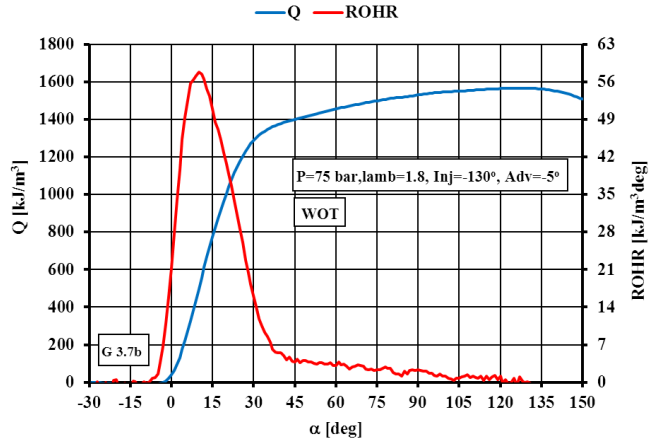

p_min
p_avg
p_max
P=75 bar,lamb=1.8, Inj=-110°, Adv=-5°
WOT
G 3.5a
p [bar]
α [deg]

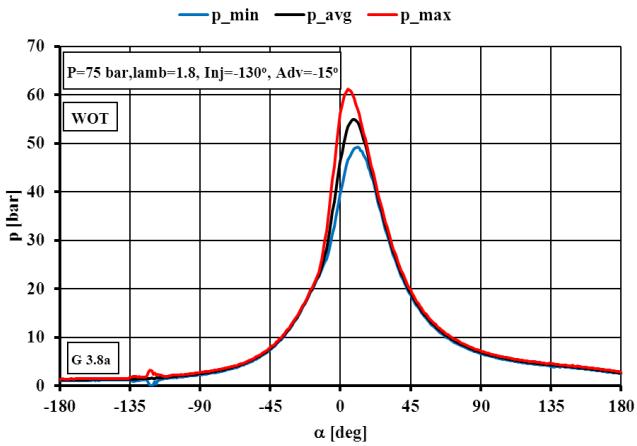

Q
ROHR
P=75 bar,lamb=1.8, Inj=-110°, Adv=-5°
WOT
G 3.5b
Q [kJ/m³]
ROHR [kJ/m³deg]
α [deg]

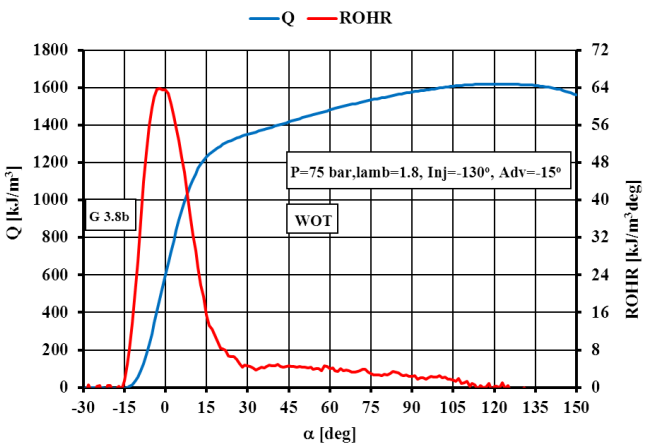

p_min
p_avg
p_max
P=75 bar,lamb=1.8, Inj=-110°, Adv=-15°
WOT
G 3.6a
p [bar]
α [deg]

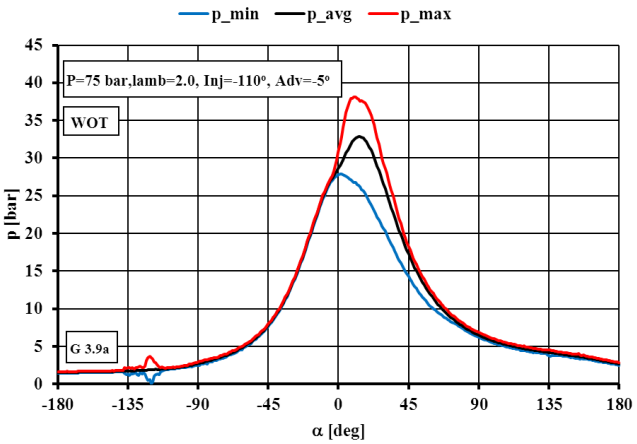

Q
ROHR
P=75 bar,lamb=1.8, Inj=-110°, Adv=-15°
WOT
G 3.6b
Q [kJ/m³]
ROHR [kJ/m³deg]
α [deg]

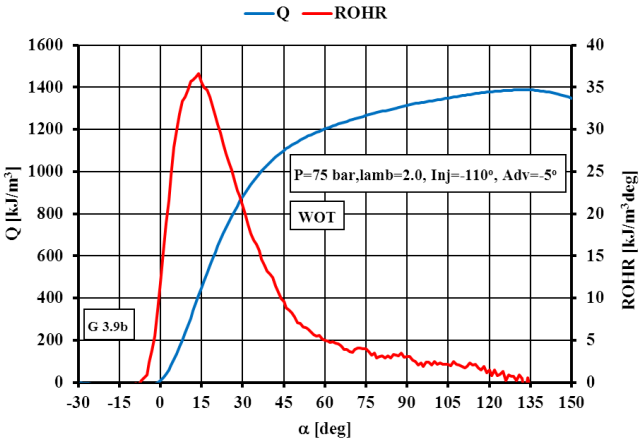

p_min
p_avg
p_max
P=75 bar,lamb=1.8, Inj=-130°, Adv=-5°
WOT
G3.7a
p [bar]
α [deg]

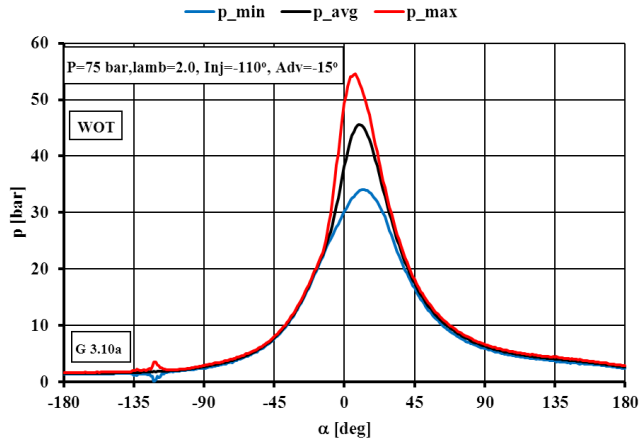

Q
ROHR
P=75 bar,lamb=1.8, Inj=-130°, Adv=-5°
WOT
G 3.7b
Q [kJ/m³]
ROHR [kJ/m³deg]
α [deg]

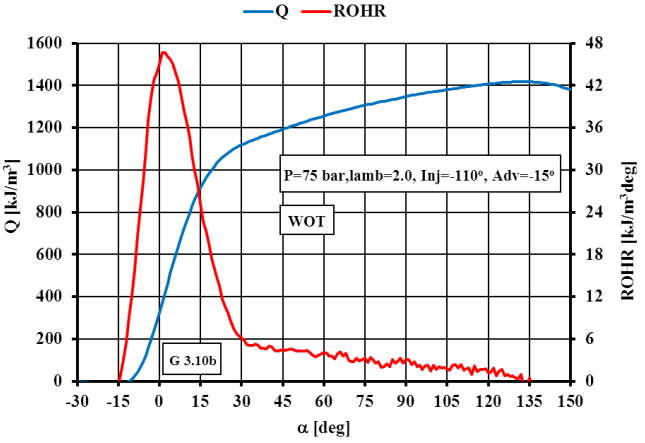

p_min
p_avg
p_max
P=75 bar,lamb=1.8, Inj=-130°, Adv=-15°
WOT
G 3.8a
p [bar]
α [deg]

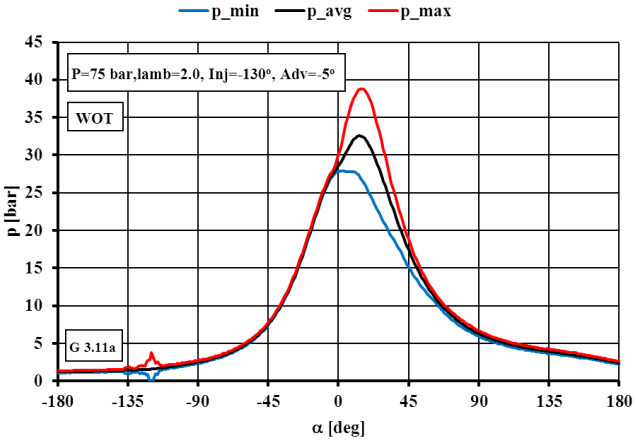

Q
ROHR
P=75 bar,lamb=1.8, Inj=-130°, Adv=-15°
WOT
G 3.8b
Q [kJ/m³]
ROHR [kJ/m³deg]
α [deg]


p_min
p_avg
p_max
P=75 bar,lamb=2.0, Inj=-110°, Adv=-5°
WOT
G 3.9a
p [bar]
α [deg]


Q
ROHR
P=75 bar,lamb=2.0, Inj=-110°, Adv=-5°
WOT
G 3.9b
Q [kJ/m³]
ROHR [kJ/m³deg]
α [deg]


p_min
p_avg
p_max
P=75 bar,lamb=2.0, Inj=-110°, Adv=-15°
WOT
G 3.10a
p [bar]
α [deg]


Q
ROHR
P=75 bar,lamb=2.0, Inj=-110°, Adv=-15°
WOT
G 3.10b
Q [kJ/m³]
ROHR [kJ/m³deg]
α [deg]


p_min
p_avg
p_max
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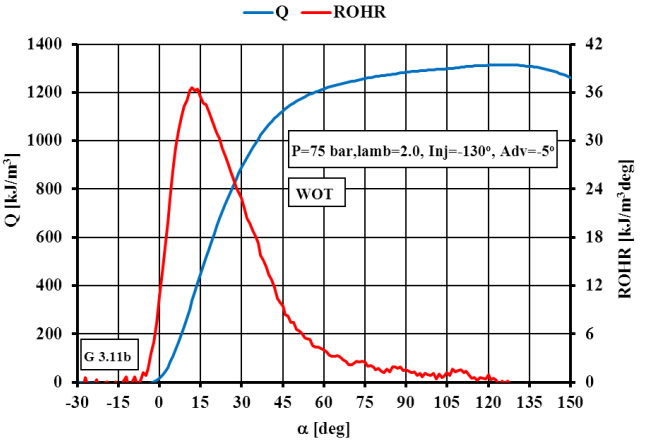
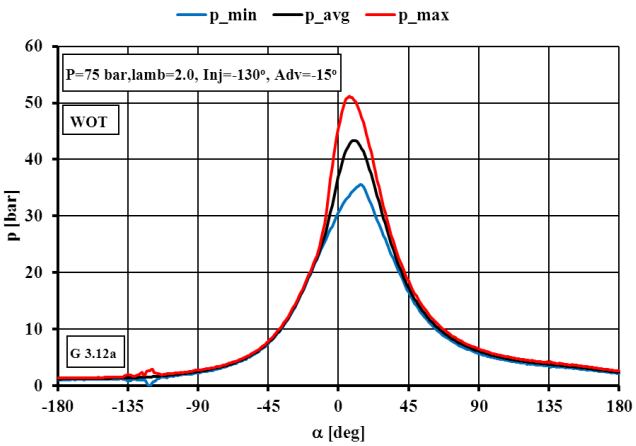
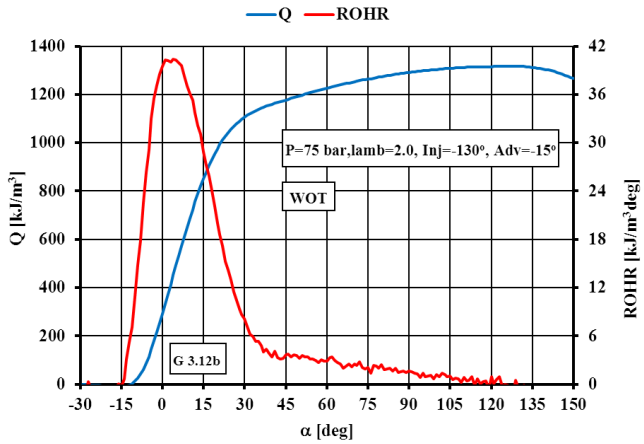
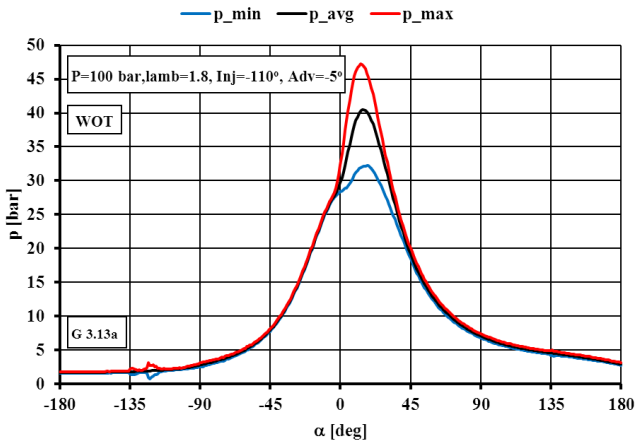
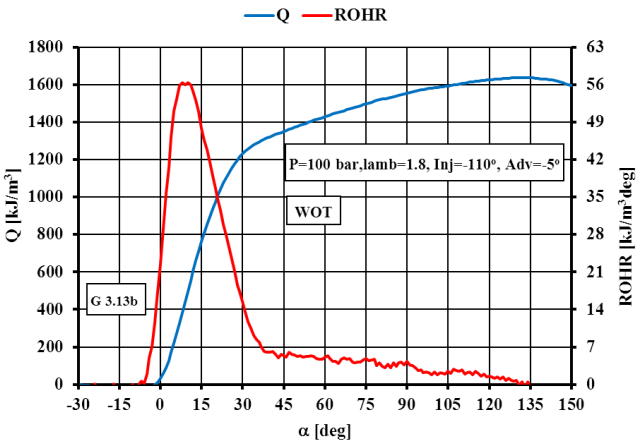
WOT
G 3.11a
p [bar]
α [deg]

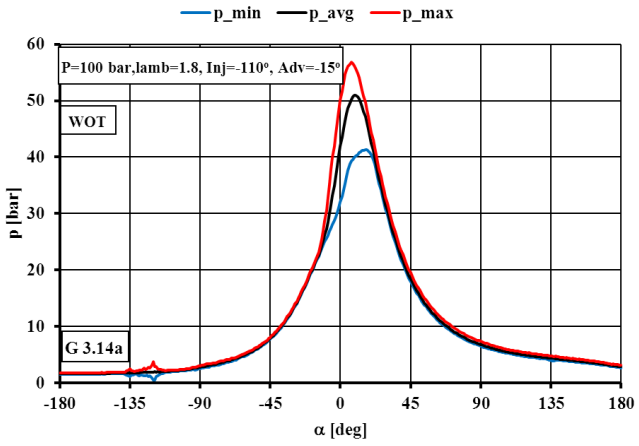

Q
ROHR
P=75 bar,lamb=2.0, Inj=-130°, Adv=-5°
WOT
G 3.11b
Q [kJ/m³]
ROHR [kJ/m³deg]
α [deg]

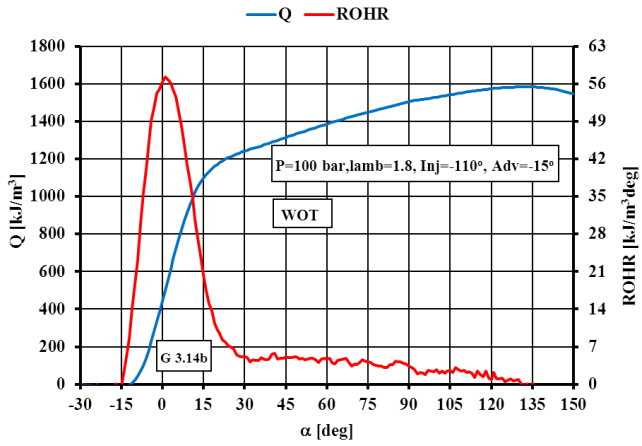

p_min
p_avg
p_max
P=75 bar,lamb=2.0, Inj=-130°, Adv=-15°
WOT
G 3.12a
p [bar]
α [deg]

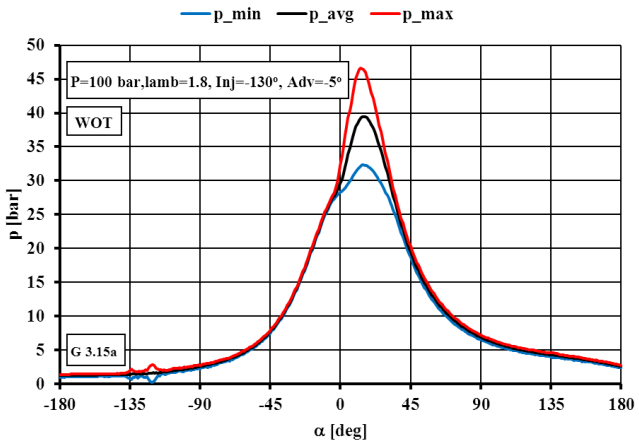

Q
ROHR
P=75 bar,lamb=2.0, Inj=-130°, Adv=-15°
WOT
G 3.12b
Q [kJ/m³]
ROHR [kJ/m³deg]
α [deg]

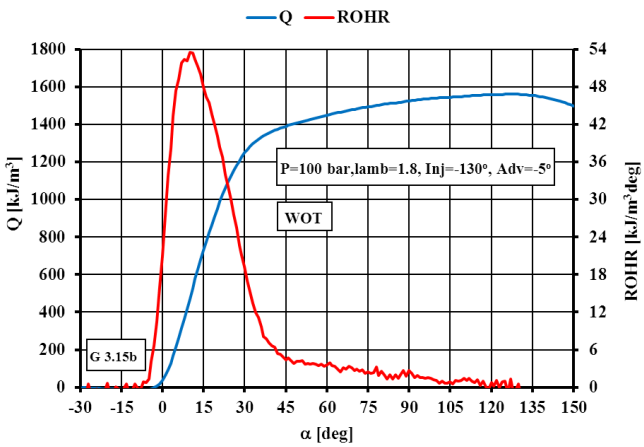

p_min
p_avg
p_max
P=100 bar,lamb=1.8, Inj=-110°, Adv=-5°
WOT
G 3.13a
p [bar]
α [deg]

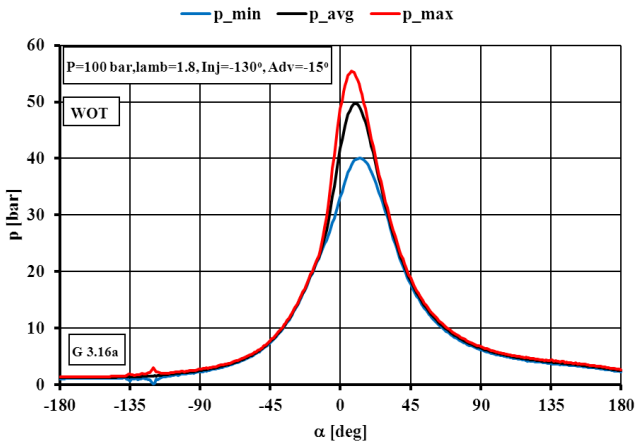

Q
ROHR
P=100 bar,lamb=1.8, Inj=-110°, Adv=-5°
WOT
G 3.13b
Q [kJ/m³]
ROHR [kJ/m³deg]
α [deg]

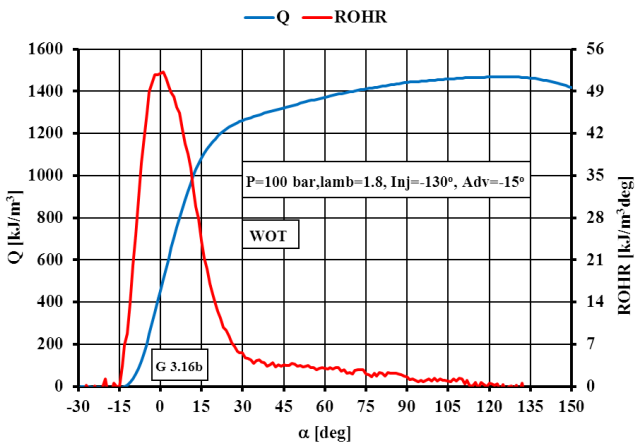

p_min
p_avg
p_max
P=100 bar,lamb=1.8, Inj=-110°, Adv=-15°
WOT
G 3.14a
p [bar]
α [deg]

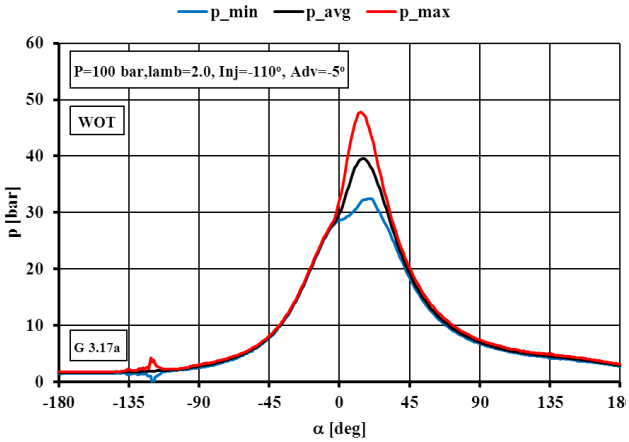

Q
ROHR
P=100 bar,lamb=1.8, Inj=-110°, Adv=-15°
WOT
G 3.14b
Q [kJ/m³]
ROHR [kJ/m³deg]
α [deg]

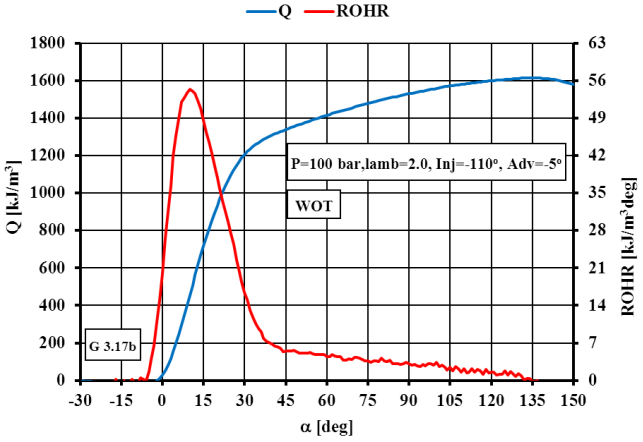

p_min
p_avg
p_max
P=100 bar,lamb=1.8, Inj=-130°, Adv=-5°
WOT
G 3.15a
p [bar]
α [deg]

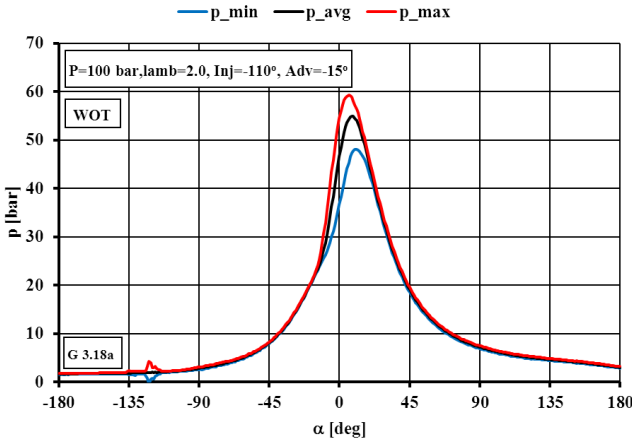

Q
ROHR
P=100 bar,lamb=1.8, Inj=-130°, Adv=-5°
WOT
G 3.15b
Q [kJ/m³]
ROHR [kJ/m³deg]
α [deg]

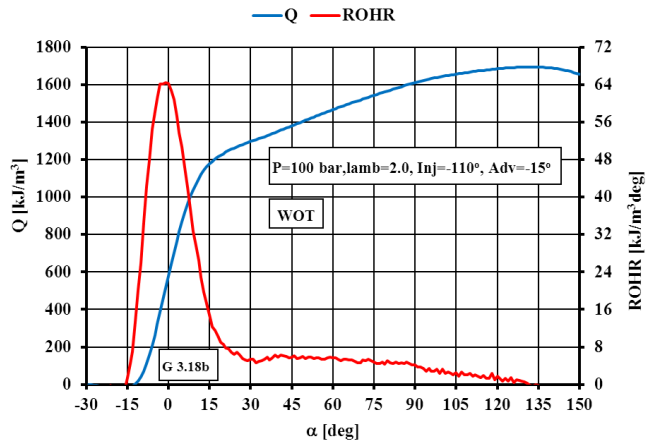

p_min
p_avg
p_max
P=100 bar,lamb=1.8, Inj=-130°, Adv=-15°
WOT
G 3.16a
p [bar]
α [deg]

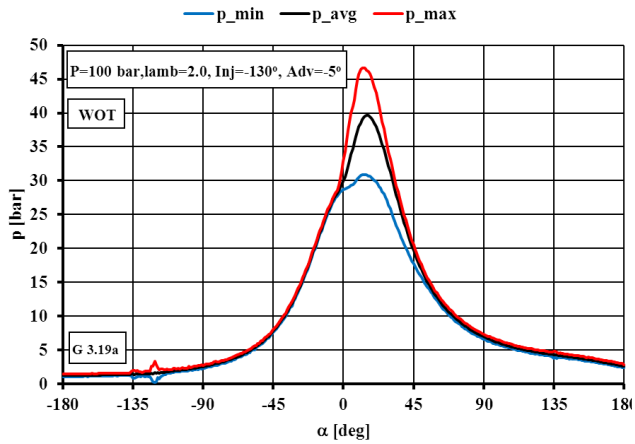

Q
ROHR
P=100 bar,lamb=1.8, Inj=-130°, Adv=-15°
WOT
G 3.16b
Q [kJ/m³]
ROHR [kJ/m³deg]
α [deg]

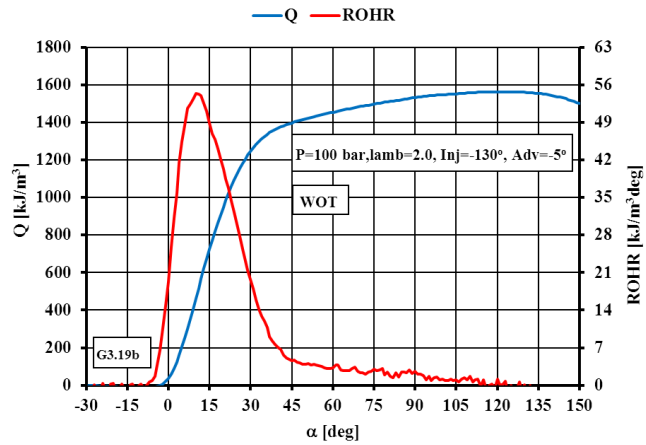

p_min
p_avg
p_max
P=100 bar,lamb=2.0, Inj=-110°, Adv=-5°
WOT
G 3.17a
p [bar]
α [deg]

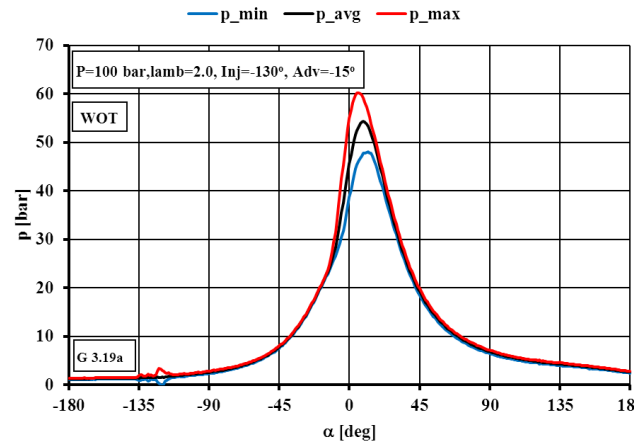

Q
ROHR
P=100 bar,lamb=2.0, Inj=-110°, Adv=-5°
WOT
G 3.17b
Q [kJ/m³]
ROHR [kJ/m³deg]
α [deg]

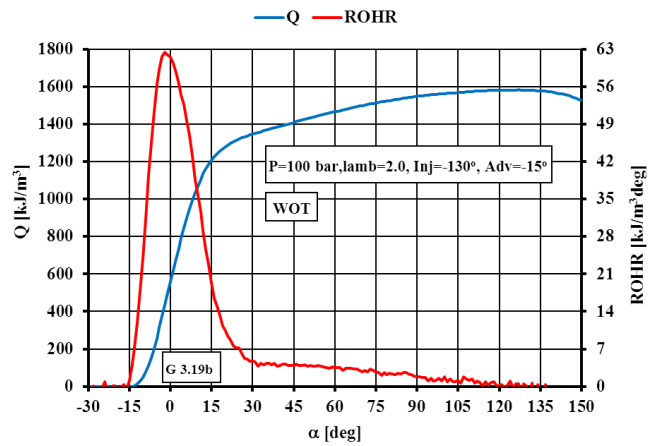

p_min
p_avg
p_max
P=100 bar,lamb=2.0, Inj=-110°, Adv=-15°
WOT
G 3.18a
p [bar]
α [deg]

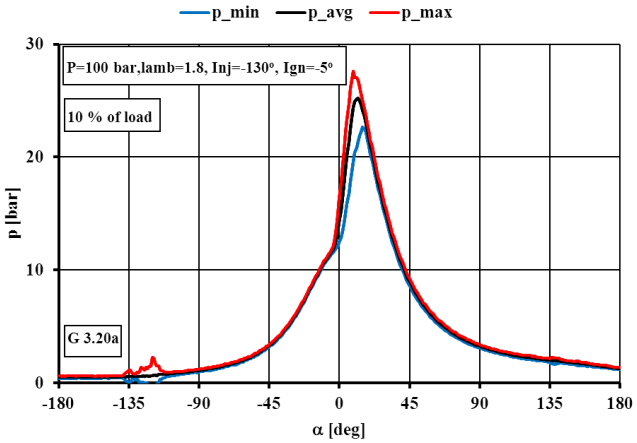

Q
ROHR
P=100 bar,lamb=2.0, Inj=-110°, Adv=-15°
WOT
G 3.18b
Q [kJ/m³]
ROHR [kJ/m³deg]
α [deg]

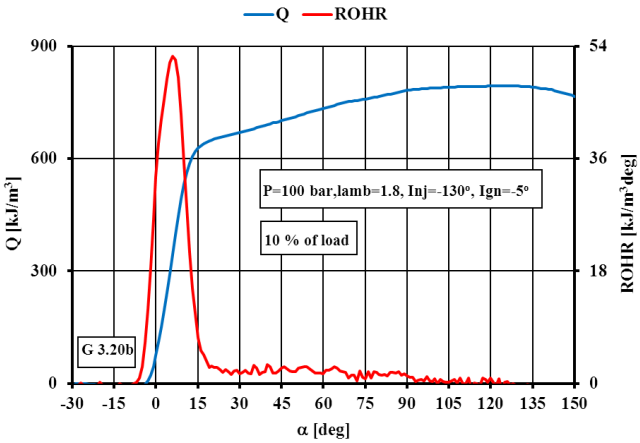

p_min
p_avg
p_max
P=100 bar,lamb=2.0, Inj=-130°, Adv=-5°
WOT
G 3.19a
p [bar]
α [deg]

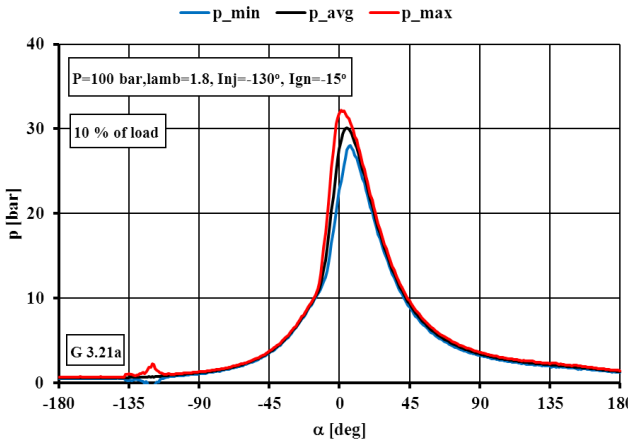

Q
ROHR
P=100 bar,lamb=2.0, Inj=-130°, Adv=-5°
WOT
G3.19b
Q [kJ/m³]
ROHR [kJ/m³deg]
α [deg]

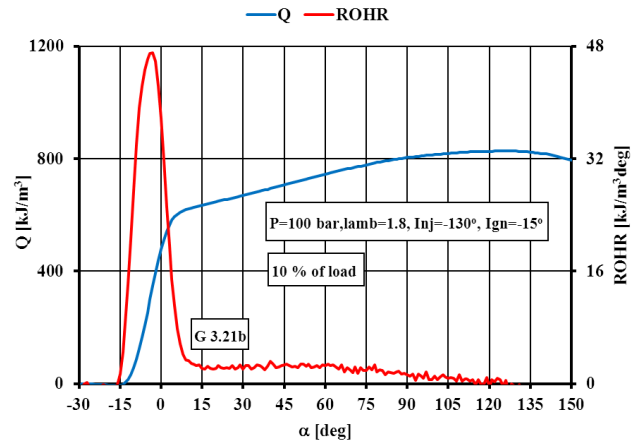

p_min
p_avg
p_max
P=100 bar,lamb=2.0, Inj=-130°, Adv=-15°
WOT
G 3.19a
p [bar]
α [deg]

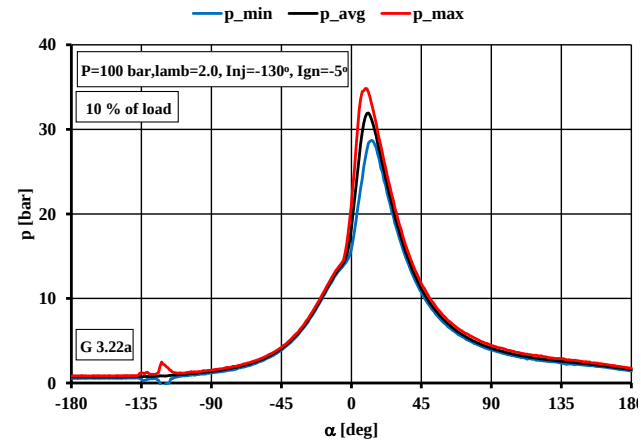

Q
ROHR
P=100 bar,lamb=2.0, Inj=-130°, Adv=-15°
WOT
G 3.19b
Q [kJ/m³]
ROHR [kJ/m³deg]
α [deg]

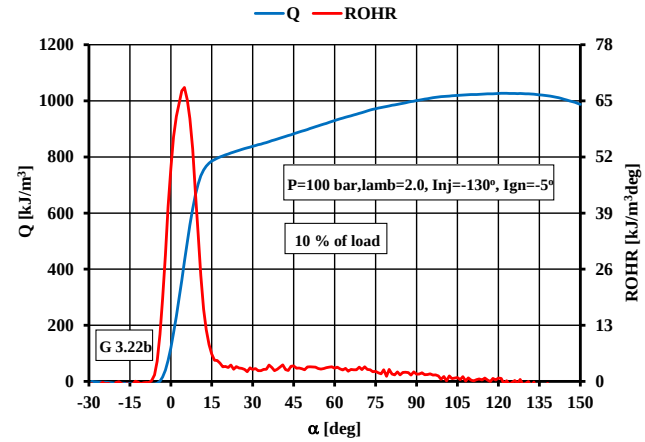

p_min
p_avg
p_max
P=100 bar,lamb=1.8, Inj=-130°, Ign=-5°
10 % of load
G 3.20a
p [bar]
α [deg]

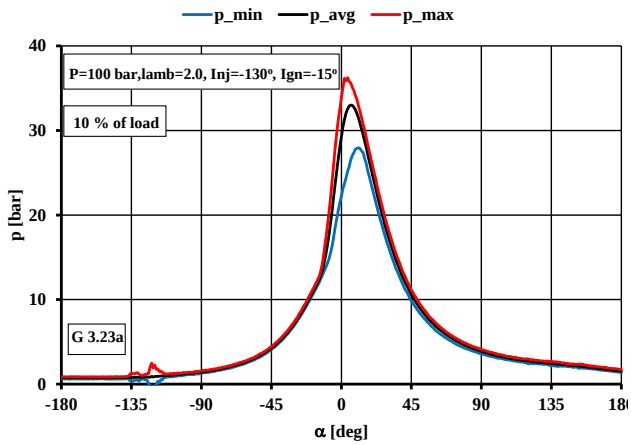

Q
ROHR
P=100 bar,lamb=1.8, Inj=-130°, Ign=-5°
10 % of load
G 3.20b
Q [kJ/m³]
ROHR [kJ/m³deg]
α [deg]

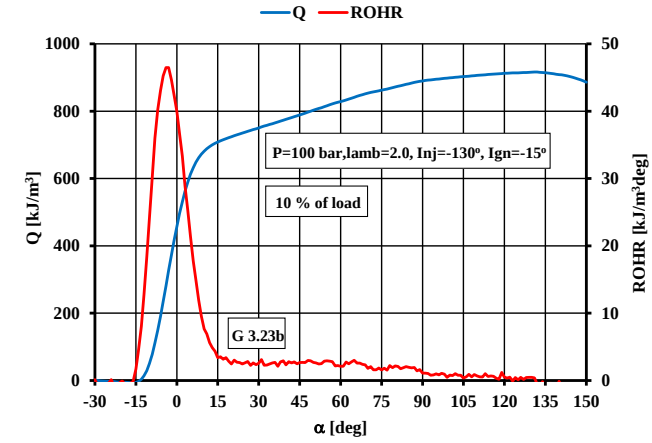

p_min
p_avg
p_max
P=100 bar,lamb=1.8, Inj=-130°, Ign=-15°
10 % of load
G 3.21a
p [bar]
α [deg]

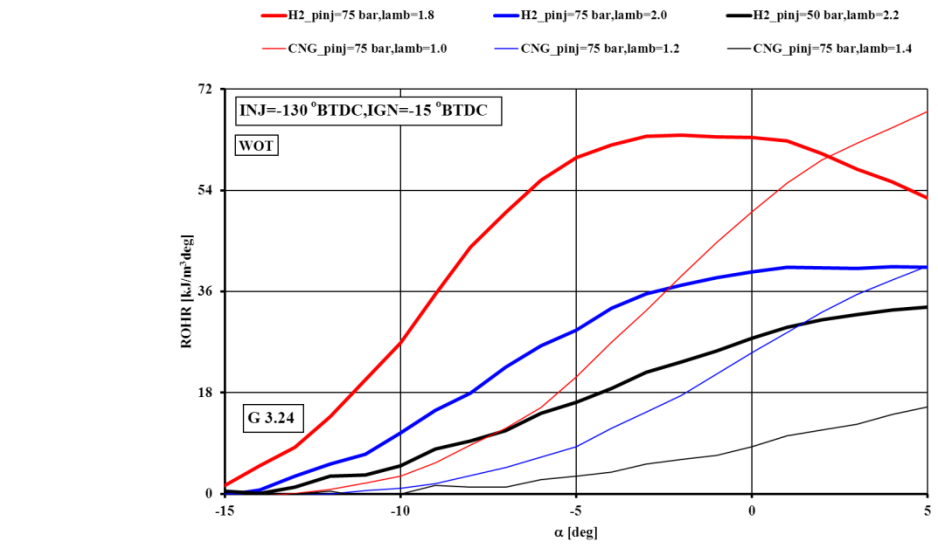

Q
ROHR
P=100 bar,lamb=1.8, Inj=-130°, Ign=-15°
10 % of load
G 3.21b
Q [kJ/m³]
ROHR [kJ/m³deg]
α [deg]

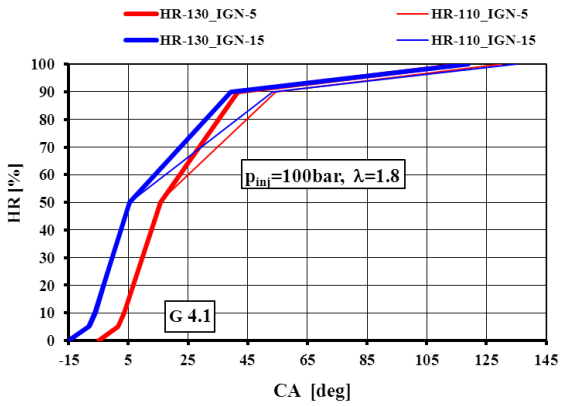

p_min
p_avg
p_max
P=100 bar,lamb=2.0, Inj=-130°, Ign=-5°
10 % of load
G 3.22a
p [bar]
α [deg]

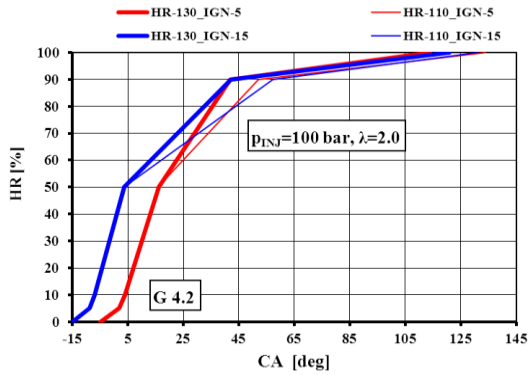

Q
ROHR
P=100 bar,lamb=2.0, Inj=-130°, Ign=-5°
10 % of load
G 3.22b
Q [kJ/m³]
ROHR [kJ/m³deg]
α [deg]

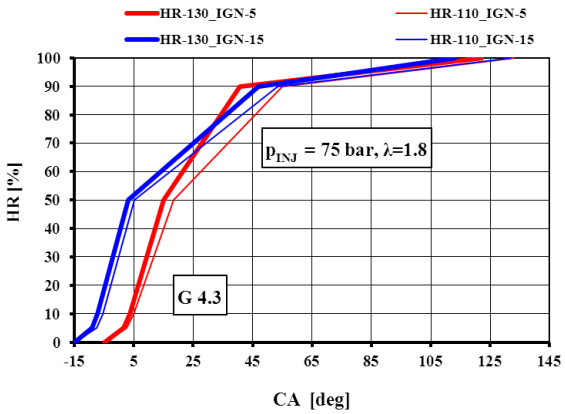

p_min
p_avg
p_max
P=100 bar,lamb=2.0, Inj=-130°, Ign=-15°
10 % of load
G 3.23a
p [bar]
α [deg]

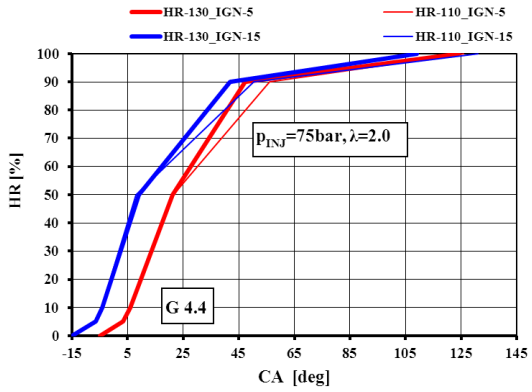

Q
ROHR
P=100 bar,lamb=2.0, Inj=-130°, Ign=-15°
10 % of load
G 3.23b
Q [kJ/m³]
ROHR [kJ/m³deg]
α [deg]

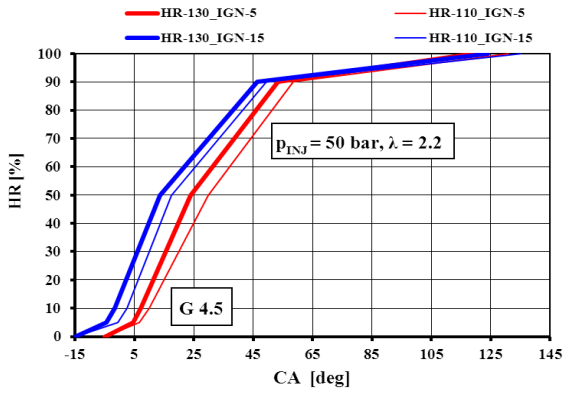

H2_pinj=75 bar,lamb=1.8
H2_pinj=75 bar,lamb=2.0
H2_pinj=50 bar,lamb=2.2
CNG_pinj=75 bar,lamb=1.0
CNG_pinj=75 bar,lamb=1.2
CNG_pinj=75 bar,lamb=1.4
INJ=-130 °BTDC,IGN=-15 °BTDC
WOT
G 3.24
ROHR [kJ/m³deg]
α [deg]

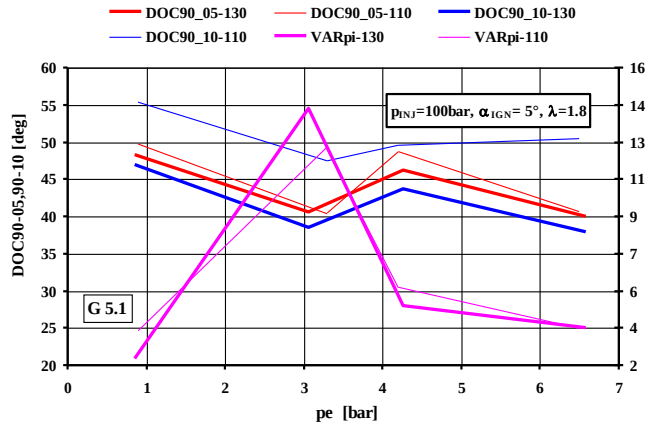

HR-130_IGN-5
HR-110_IGN-5
HR-130_IGN-15
HR-110_IGN-15
p_inj=100bar, λ=1.8
G 4.1
HR [%]
CA [deg]

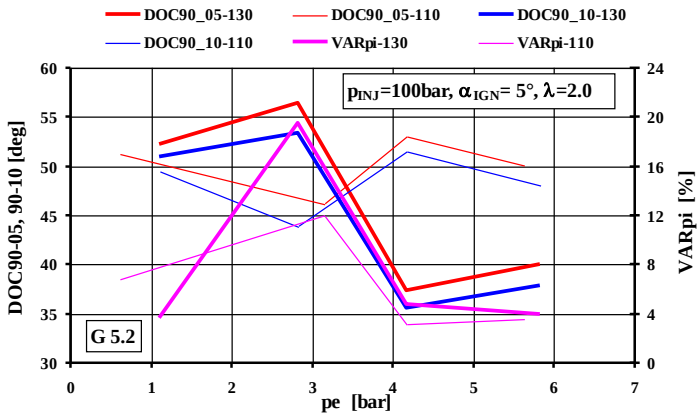

HR-130_IGN-5
HR-110_IGN-5
HR-130_IGN-15
HR-110_IGN-15
p_INJ=100 bar, λ=2.0
G 4.2
HR [%]
CA [deg]

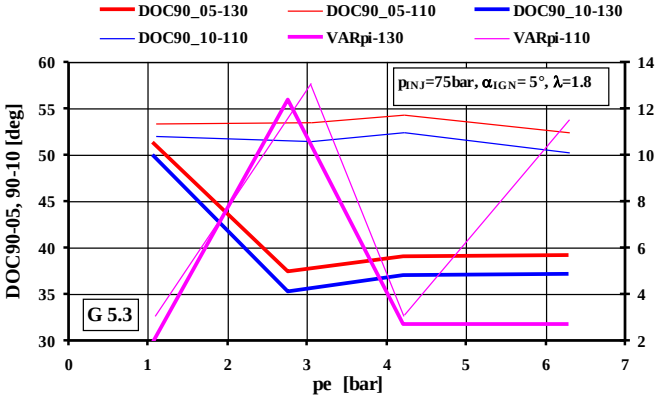

HR-130_IGN-5
HR-110_IGN-5
HR-130_IGN-15
HR-110_IGN-15
p_INJ = 75 bar, λ=1.8
G 4.3
HR [%]
CA [deg]

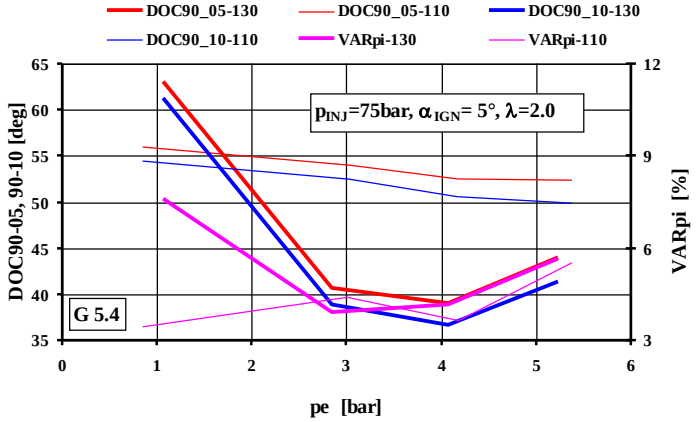

HR-130_IGN-5
HR-110_IGN-5
HR-130_IGN-15
HR-110_IGN-15
p_INJ=75bar, λ=2.0
G 4.4
HR [%]
CA [deg]

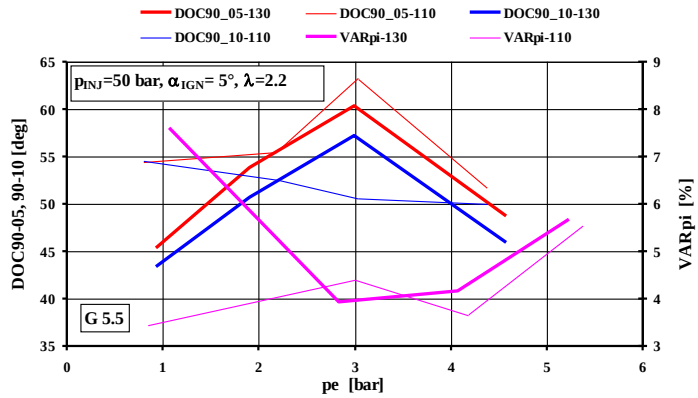

HR-130_IGN-5
HR-110_IGN-5
HR-130_IGN-15
HR-110_IGN-15
p_INJ = 50 bar, λ = 2.2
G 4.5
HR [%]
CA [deg]

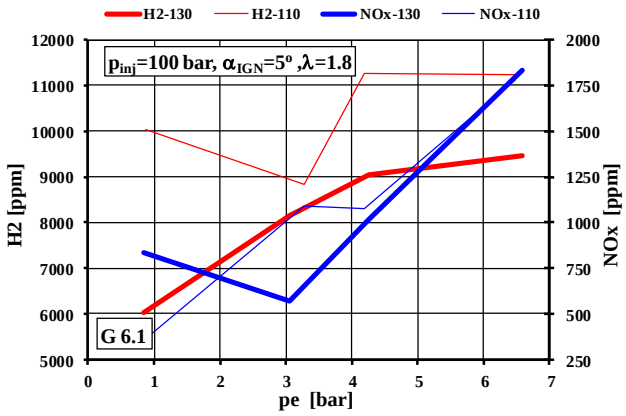

DOC90_05-130
DOC90_05-110
DOC90_10-130
DOC90_10-110
VARpi-130
VARpi-110
pINJ=100bar, αIGN= 5°, λ=1.8
G 5.1
DOC90-05,90-10 [deg]
VARpi [%]
pe [bar]

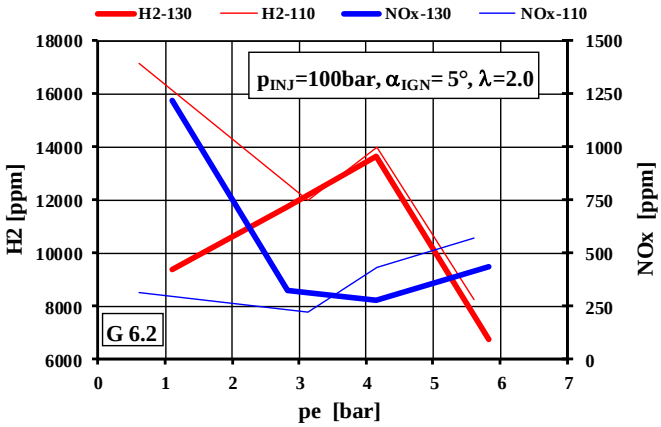

DOC90_05-130
DOC90_05-110
DOC90_10-130
DOC90_10-110
VARpi-130
VARpi-110
pINJ=100bar, αIGN= 5°, λ=2.0
G 5.2
DOC90-05, 90-10 [deg]
VARpi [%]
pe [bar]

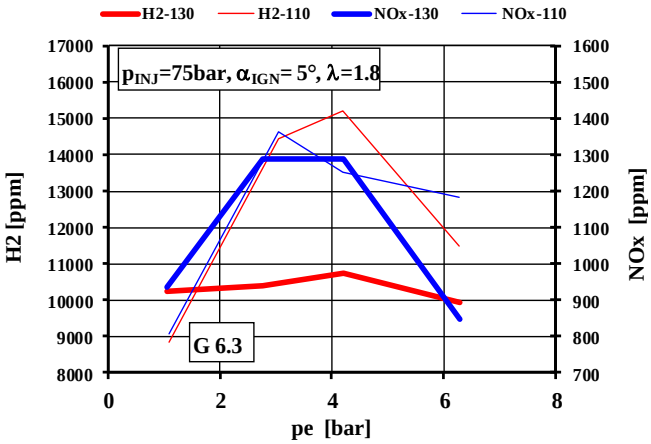

DOC90_05-130
DOC90_05-110
DOC90_10-130
DOC90_10-110
VARpi-130
VARpi-110
pINJ=75bar, αIGN= 5°, λ=1.8
G 5.3
DOC90-05, 90-10 [deg]
VARpi [%]
pe [bar]

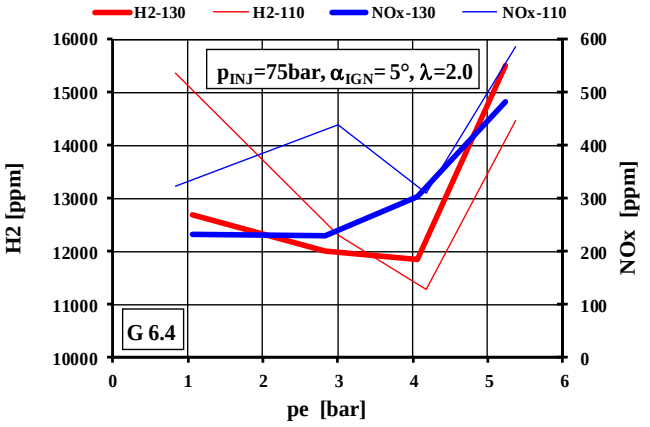

DOC90_05-130
DOC90_05-110
DOC90_10-130
DOC90_10-110
VARpi-130
VARpi-110
pINJ=75bar, αIGN= 5°, λ=2.0
G 5.4
DOC90-05, 90-10 [deg]
VARpi [%]
pe [bar]

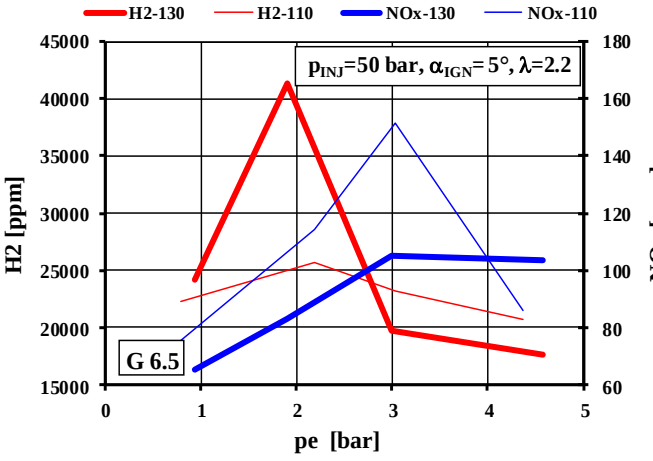

DOC90_05-130
DOC90_05-110
DOC90_10-130
DOC90_10-110
VARpi-130
VARpi-110
pINJ=50 bar, αIGN= 5°, λ=2.2
G 5.5
DOC90-05, 90-10 [deg]
VARpi [%]
pe [bar]

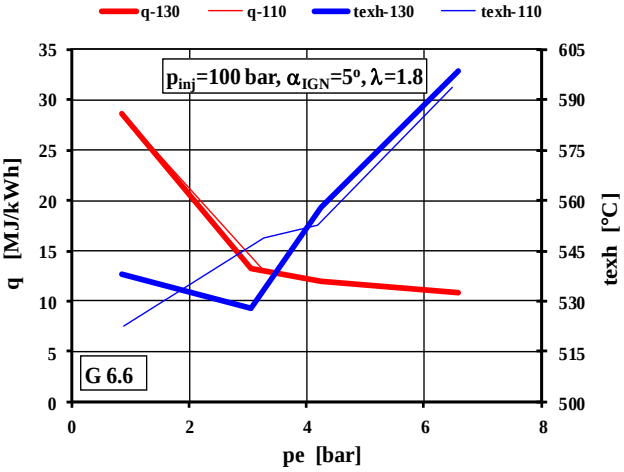

H2-130
H2-110
NOx-130
NOx-110
p_{inj}=100 bar, α_{IGN}=5° ,λ=1.8
G 6.1
H2 [ppm]
NOx [ppm]
pe [bar]

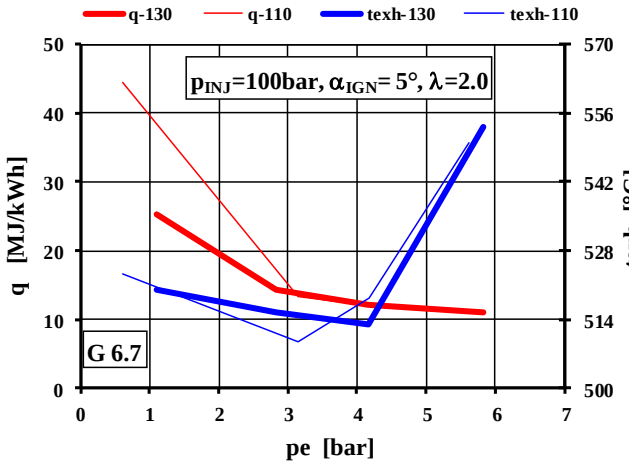

H2-130
H2-110
NOx-130
NOx-110
p_{INJ}=100bar, α_{IGN}= 5°, λ=2.0
G 6.2
H2 [ppm]
NOx [ppm]
pe [bar]

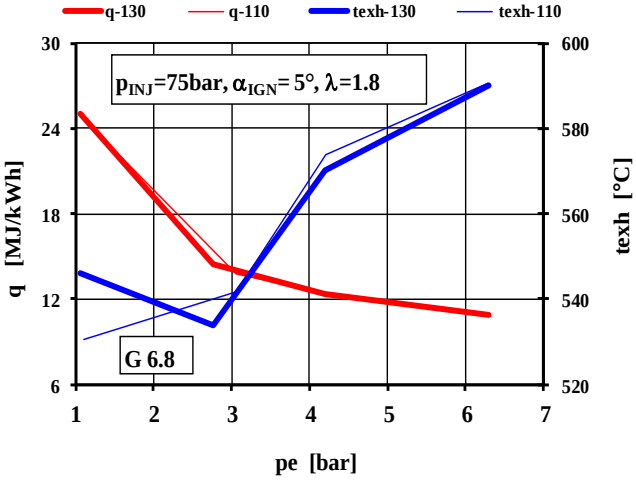

H2-130
H2-110
NOx-130
NOx-110
p_{INJ}=75bar, α_{IGN}= 5°, λ=1.8
G 6.3
H2 [ppm]
NOx [ppm]
pe [bar]

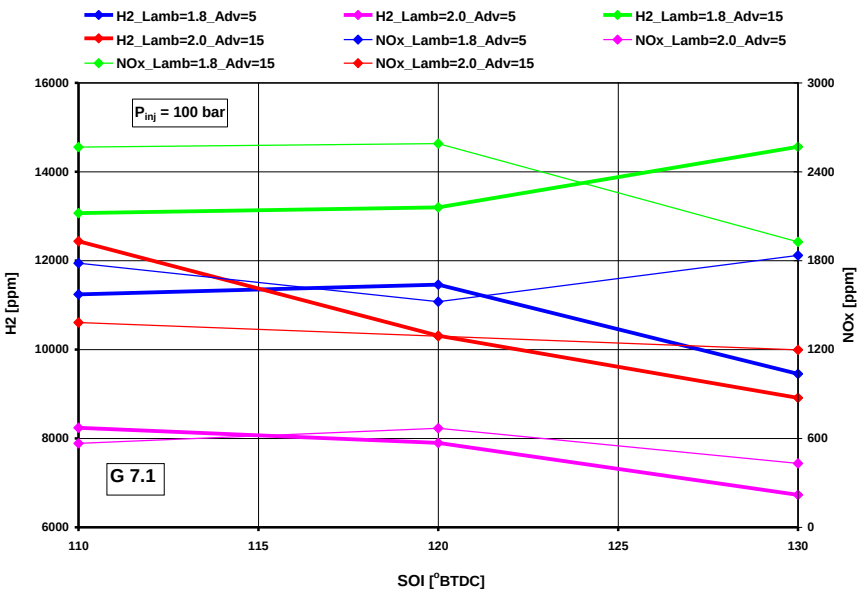

H2-130
H2-110
NOx-130
NOx-110
p_{INJ}=75bar, α_{IGN}= 5°, λ=2.0
G 6.4
H2 [ppm]
NOx [ppm]
pe [bar]

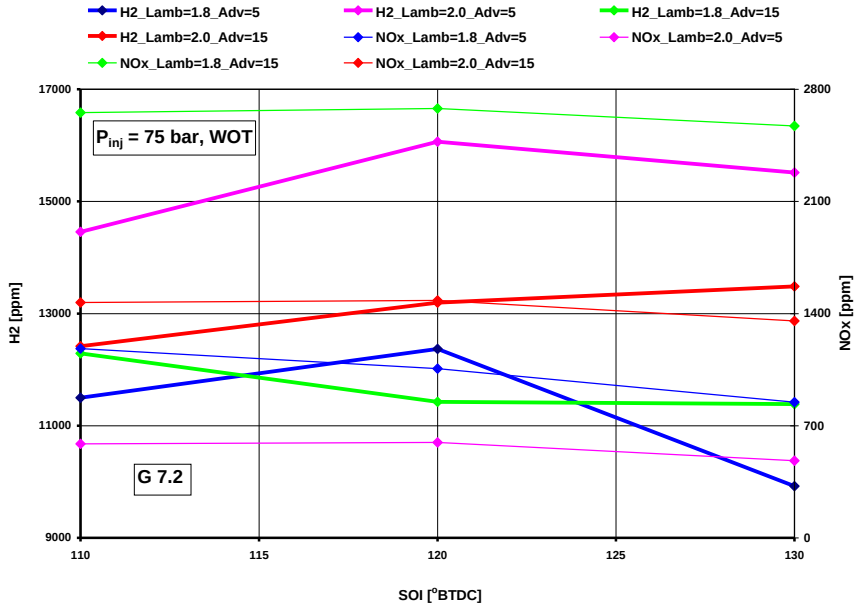

H2-130
H2-110
NOx-130
NOx-110
p_{INJ}=50 bar, α_{IGN}= 5°, λ=2.2
G 6.5
H2 [ppm]
NOx [ppm]
pe [bar]

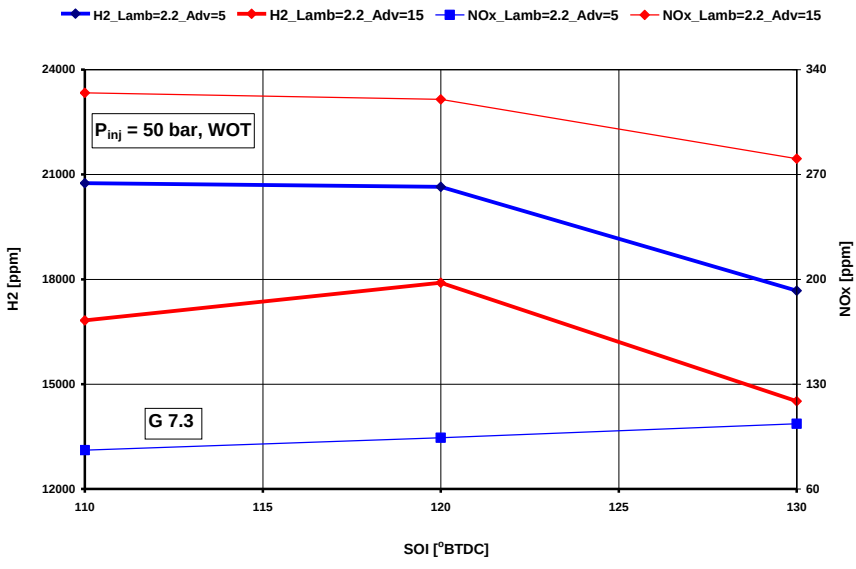

q-130
q-110
texh-130
texh-110
p_{inj}=100 bar, α_{IGN}=5°, λ=1.8
G 6.6
q [MJ/kWh]
texh [°C]
pe [bar]

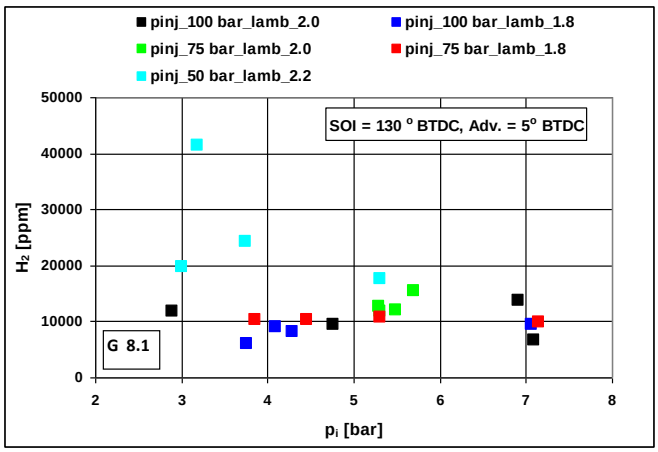

q-130
q-110
texh-130
texh-110
p_{INJ}=100bar, α_{IGN}= 5°, λ=2.0
G 6.7
q [MJ/kWh]
texh [°C]
pe [bar]


q-130
q-110
texh-130
texh-110
p_{INJ}=75bar, α_{IGN}= 5°, λ=1.8
G 6.8
q [MJ/kWh]
texh [°C]
pe [bar]


H2_Lamb=1.8_Adv=5
H2_Lamb=2.0_Adv=5
H2_Lamb=1.8_Adv=15
H2_Lamb=2.0_Adv=15
NOx_Lamb=1.8_Adv=5
NOx_Lamb=2.0_Adv=5
NOx_Lamb=1.8_Adv=15
NOx_Lamb=2.0_Adv=15
P_inj = 100 bar
G 7.1
H2 [ppm]
NOx [ppm]
SOI [°BTDC]


H2_Lamb=1.8_Adv=5
H2_Lamb=2.0_Adv=5
H2_Lamb=1.8_Adv=15
H2_Lamb=2.0_Adv=15
NOx_Lamb=1.8_Adv=5
NOx_Lamb=2.0_Adv=5
NOx_Lamb=1.8_Adv=15
NOx_Lamb=2.0_Adv=15
P_inj = 75 bar, WOT
G 7.2
H2 [ppm]
NOx [ppm]
SOI [°BTDC]


H2_Lamb=2.2_Adv=5
H2_Lamb=2.2_Adv=15
NOx_Lamb=2.2_Adv=5
NOx_Lamb=2.2_Adv=15
P_inj = 50 bar, WOT
G 7.3
H2 [ppm]
NOx [ppm]
SOI [°BTDC]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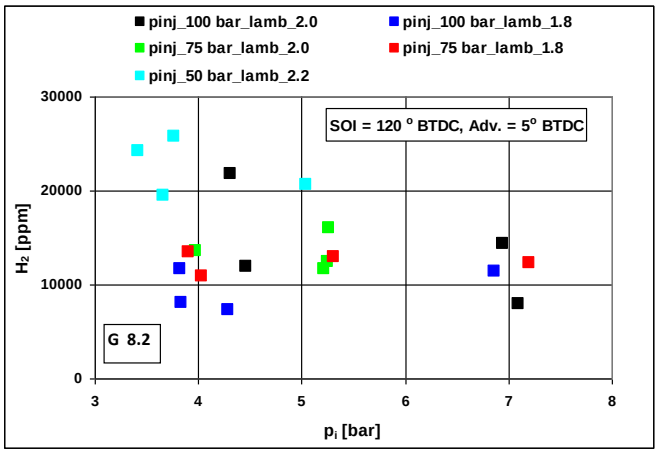
H2 [ppm]
pi [bar]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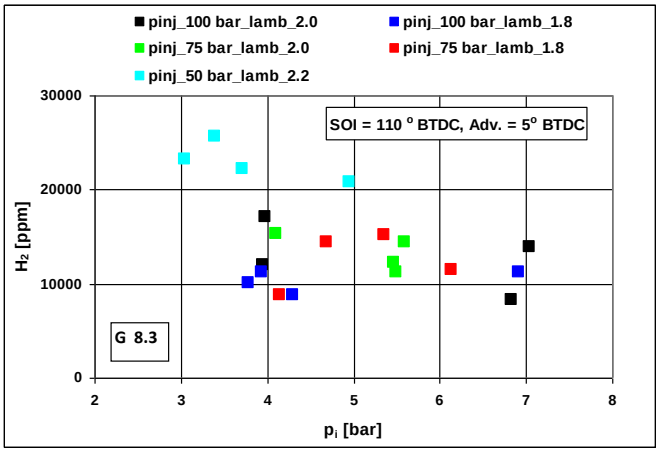
pi [bar]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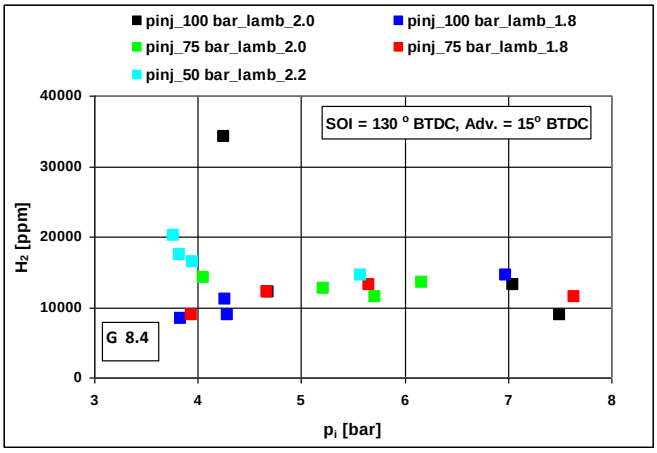
H2 [ppm]
pi [bar]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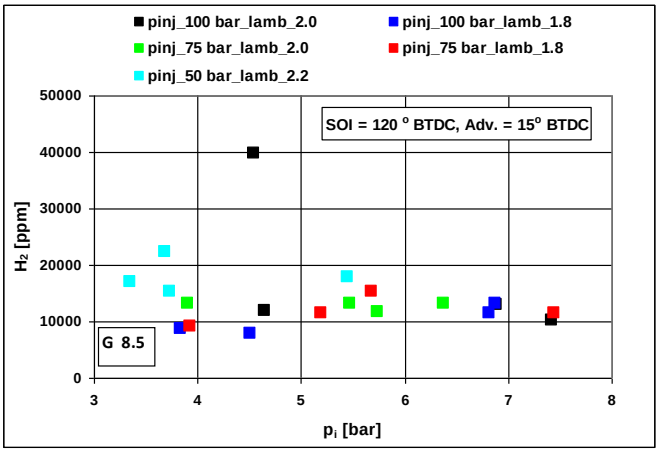
pi [bar]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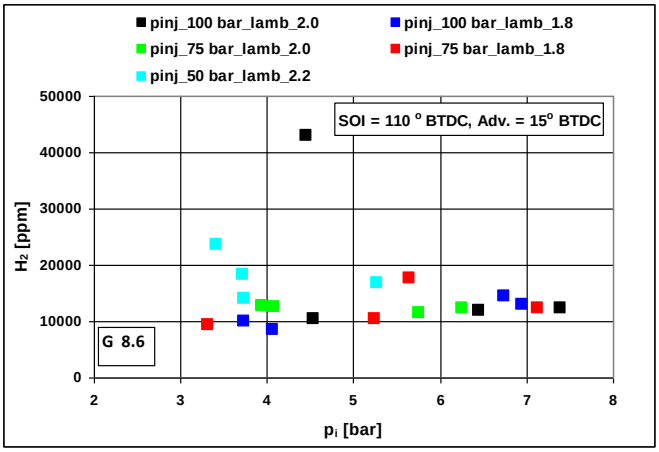
H2 [ppm]
pi [bar]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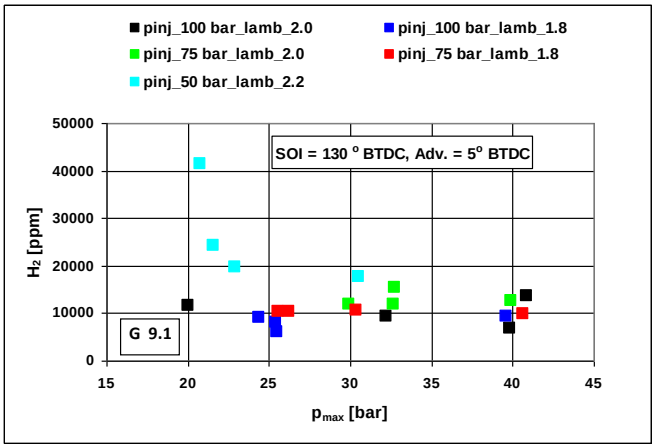
H2 [ppm]
pi [bar]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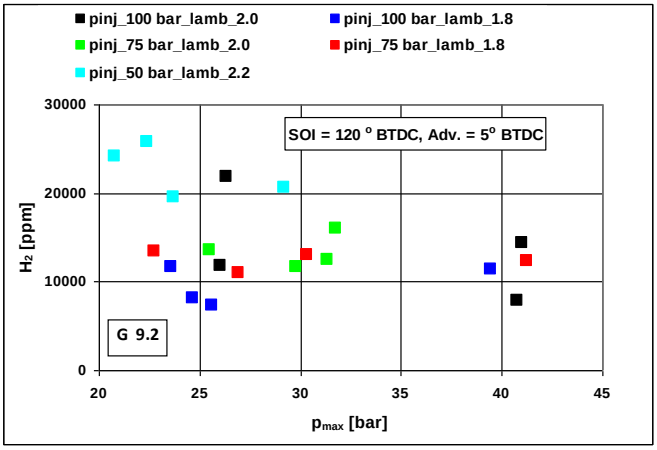
H₂ [ppm]
pmax [bar]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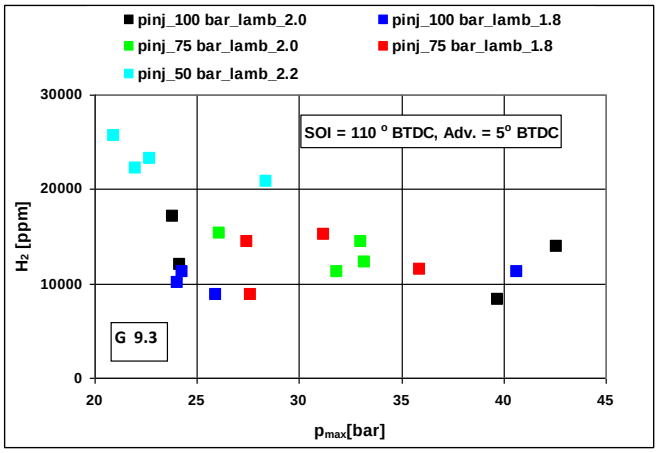
H₂ [ppm]
pmax [bar]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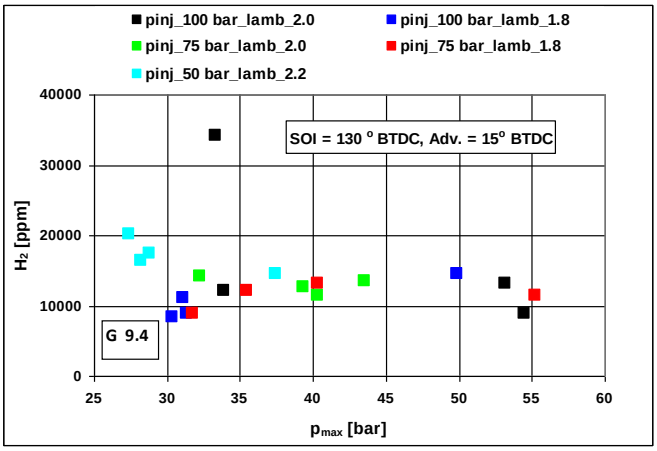
G 9.3
H₂ [ppm]
pmax[bar]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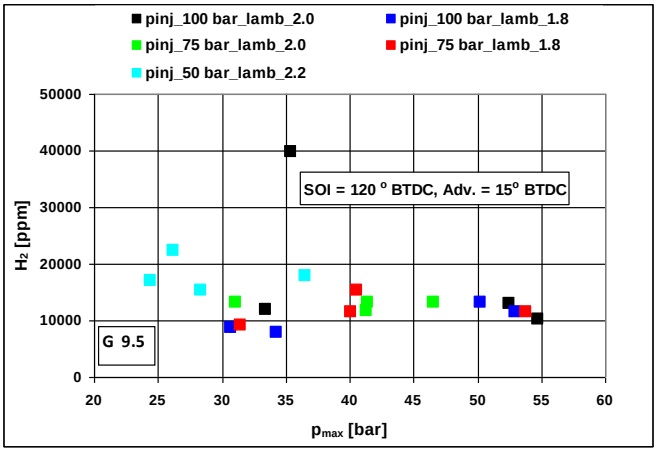
H₂ [ppm]
pmax [bar]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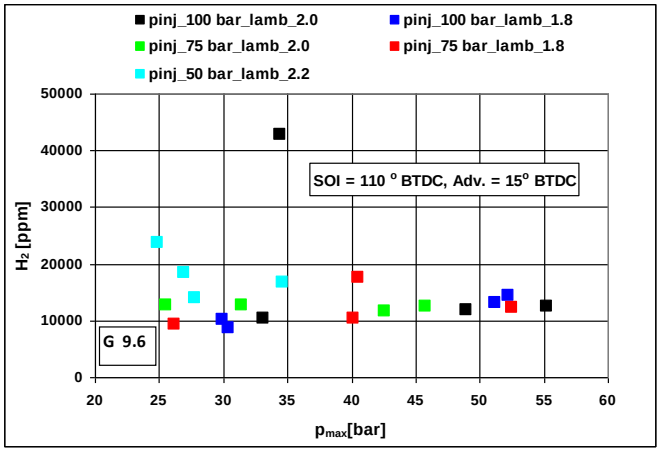
G 9.5
H₂ [ppm]
pmax [bar]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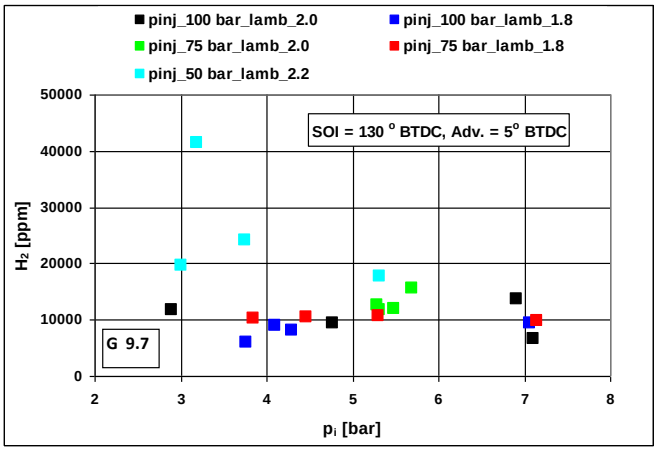
G 9.6
H₂ [ppm]
pmax[bar]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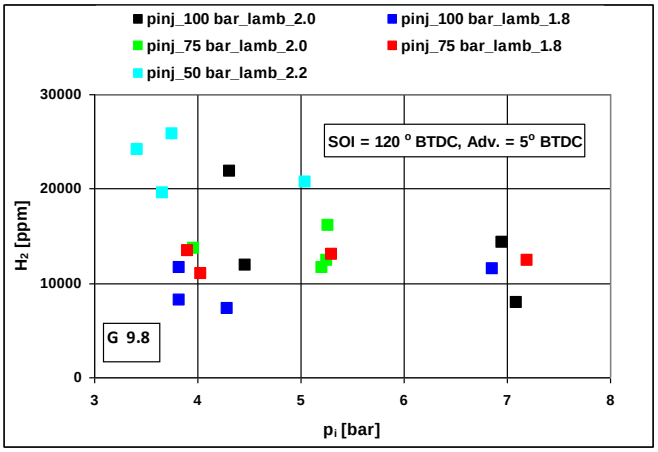
G 9.7
H2 [ppm]
pi [bar]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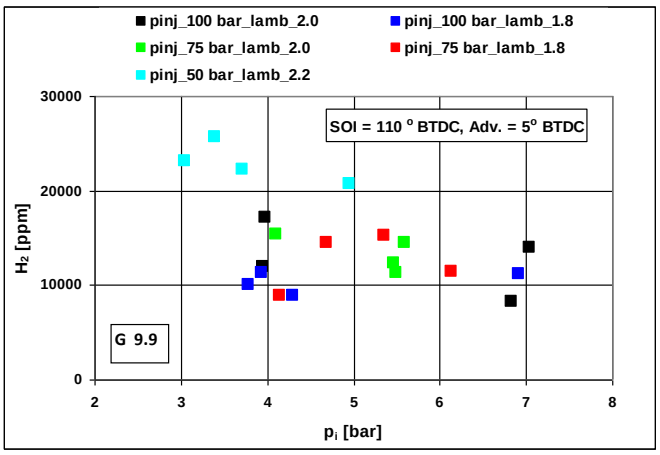
G 9.8
H2 [ppm]
pi [bar]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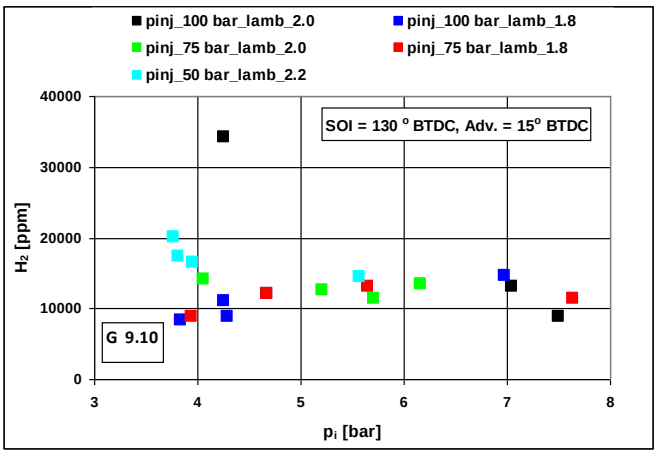
SOI = 110 ° BTDC, Adv. = 5° BTDC
G 9.9
H2 [ppm]
pi [bar]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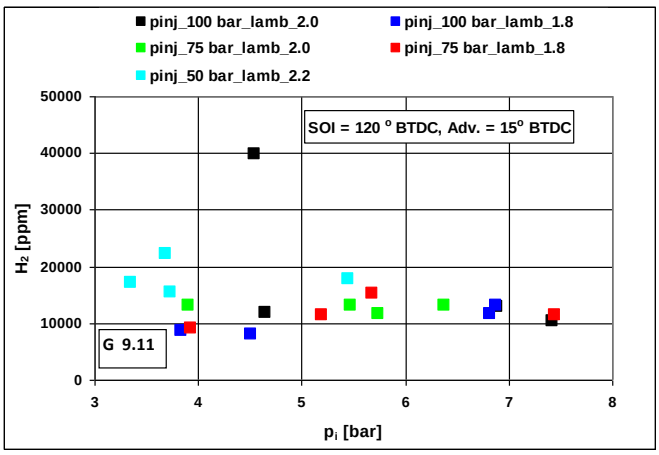
SOI = 130 ° BTDC, Adv. = 15° BTDC
G 9.10
H2 [ppm]
pi [bar]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pinj_75 bar_lamb_1.8
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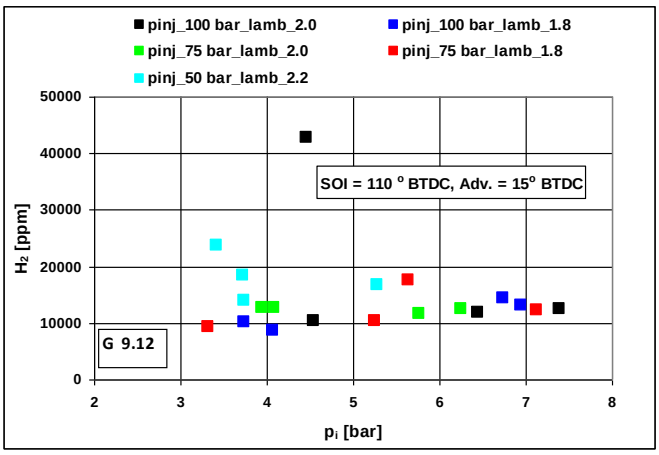
SOI = 120 ° BTDC, Adv. = 15° BTDC
G 9.11
H2 [ppm]
pi [bar]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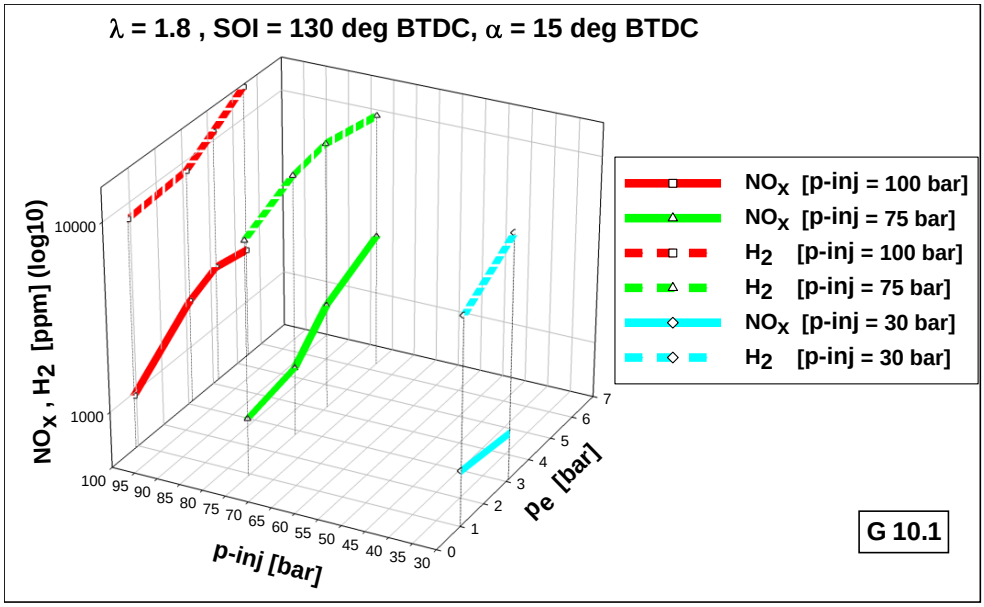
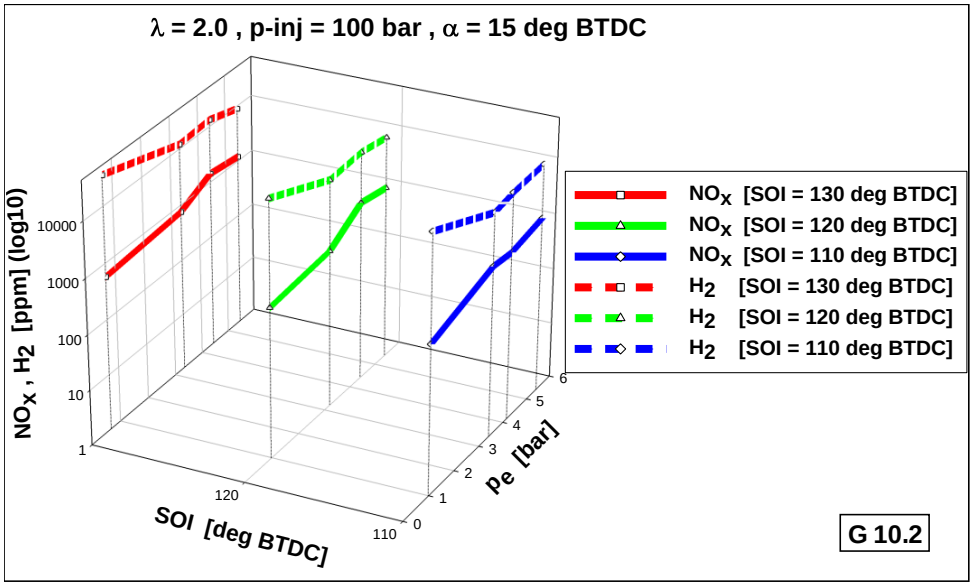
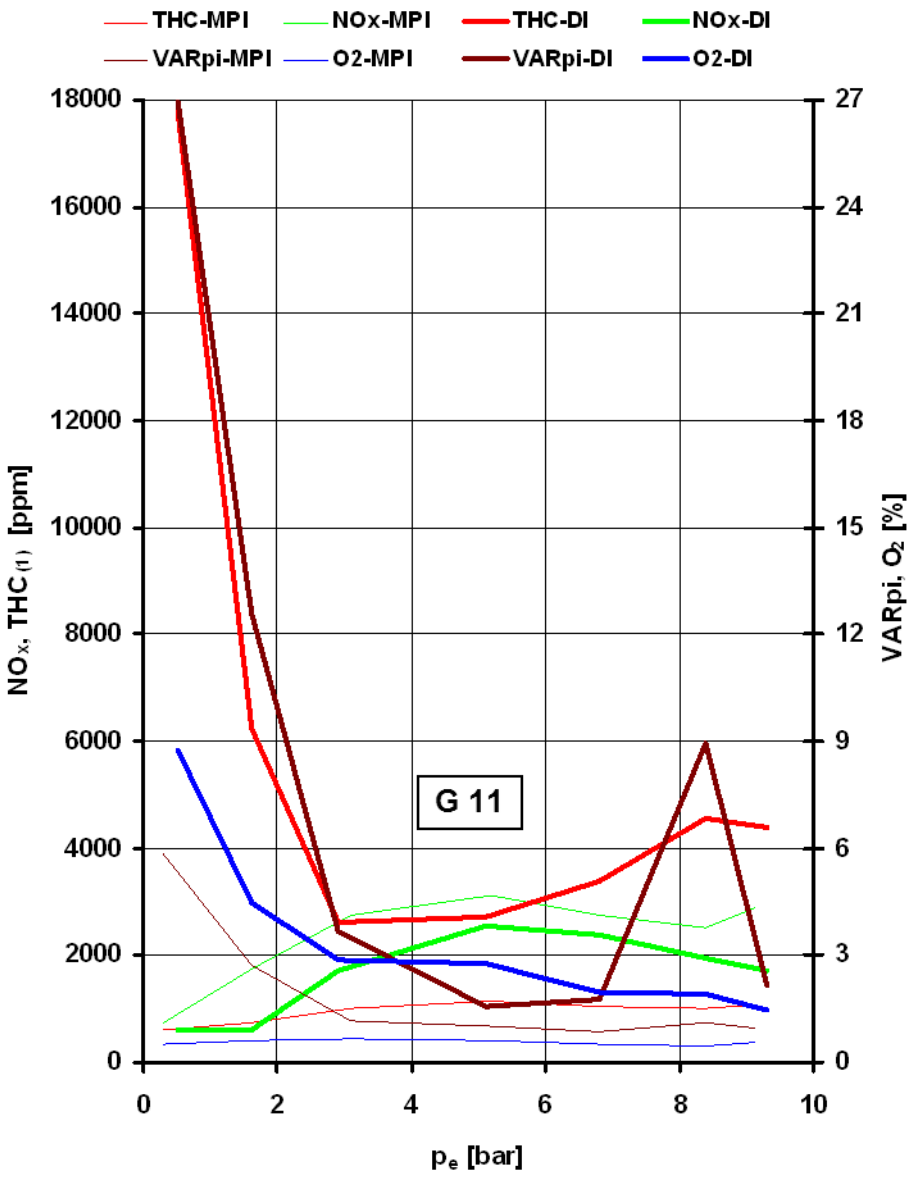
SOI = 110 ° BTDC, Adv. = 15° BTDC
G 9.12
H2 [ppm]
pi [bar]


λ = 1.8 , SOI = 130 deg BTDC, α = 15 deg BTDC
NOX , H2 [ppm] (log10)
10000
1000
100
95 90 85 80 75 70 65 60 55 50 45 40 35 30
p-inj [bar]
0 1 2 3 4 5 6 7
Pe [bar]
NOX [p-inj = 100 bar]
NOX [p-inj = 75 bar]
H2 [p-inj = 100 bar]
H2 [p-inj = 75 bar]
NOX [p-inj = 30 bar]
H2 [p-inj = 30 bar]
G 10.1


λ = 2.0 , p-inj = 100 bar , α = 15 deg BTDC
NOX , H2 [ppm] (log10)
10000
1000
100
10
1
120
SOI [deg BTDC]
110
0 1 2 3 4 5 6
Pe [bar]
NOX [SOI = 130 deg BTDC]
NOX [SOI = 120 deg BTDC]
NOX [SOI = 110 deg BTDC]
H2 [SOI = 130 deg BTDC]
H2 [SOI = 120 deg BTDC]
H2 [SOI = 110 deg BTDC]
G 10.2


THC-MPI
NOx-MPI
THC-DI
NOx-DI
VARpi-MPI
O2-MPI
VARpi-DI
O2-DI
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
27
24
21
18
15
12
9
6
3
0
0
2
4
6
8
10
NOx, THC(1) [ppm]
VARpi, O2 [%]
pe [bar]
G 11

APPENDIX 2

Description the methods for calculation of NO_x formation in cylinder by combustion[45]

The NO production is dependent namely on local temperature, on the time abidance of nitrogen molecule in the area with the high temperature and on the oxygen concentration: the decreasing of NO creating is possible to influence first of all by decreasing of temperature of the mixture combusted. The decisive influence on the NO production has the course of combustion process, which designates the distribution and the magnitude of temperature in the progress of working cycle.

The oxidation of atmospheric nitrogen at the combustion of fuel-air mixture schematically describe the Zeldovich mechanism, so-called thermal process of NO creation: the significant influence on the mechanism of NO creation they have the concentration of atomic nitrogen and atomic oxygen, which are as results of the molecule decomposition of N_2 and O_2 by effects of high temperature in the area of burning and at area of exhaust gas with the high temperature.

$$\mathbf{O + N_2 \leftrightarrow NO + N} \quad (1)$$

$$\mathbf{N + O_2 \leftrightarrow NO + O} \quad (2)$$

$$\mathbf{N + OH \leftrightarrow NO + H} \quad (3)$$

Necessary condition for the reaction process is the high temperature (> 1000 ^{0}C). The reaction (1) and (2) they are meaningful at the combustion of stoichiometric or poor mixture; the reactions (1) and (3) are important at the combustion of rich mixture, the reaction (2) at this case is a high suppression for the low concentration of oxygen. On the whole procedure of NO creation it is necessary regard like on process, which has the dynamically progress during time. These reactions are in progress from the initial rise of flame to full burn-up of mixture with the resulting by the instrumentality of high temperature of the burning gas on that reactant N_2 and O_2.

For the calculation of NO production it is needed to determine the courses of temperature in the individual volumetric element in cylinder charge according to time of their burn-up. The simulation model for the calculation of gradual burn-up of cylinder charge by separate layers has been presented in [43], the result of the calculation shows figure 1. The whole mass cylinder charge is distributed to 10 layers, whose the mass sizes they are determined by quantity of heat, that will be delivered at their gradual burn-up (determined by Wiebe equation for burning of cylinder charge): the burning time (angle of angular rotation of crankshaft) has the identical size for every 10 layers.

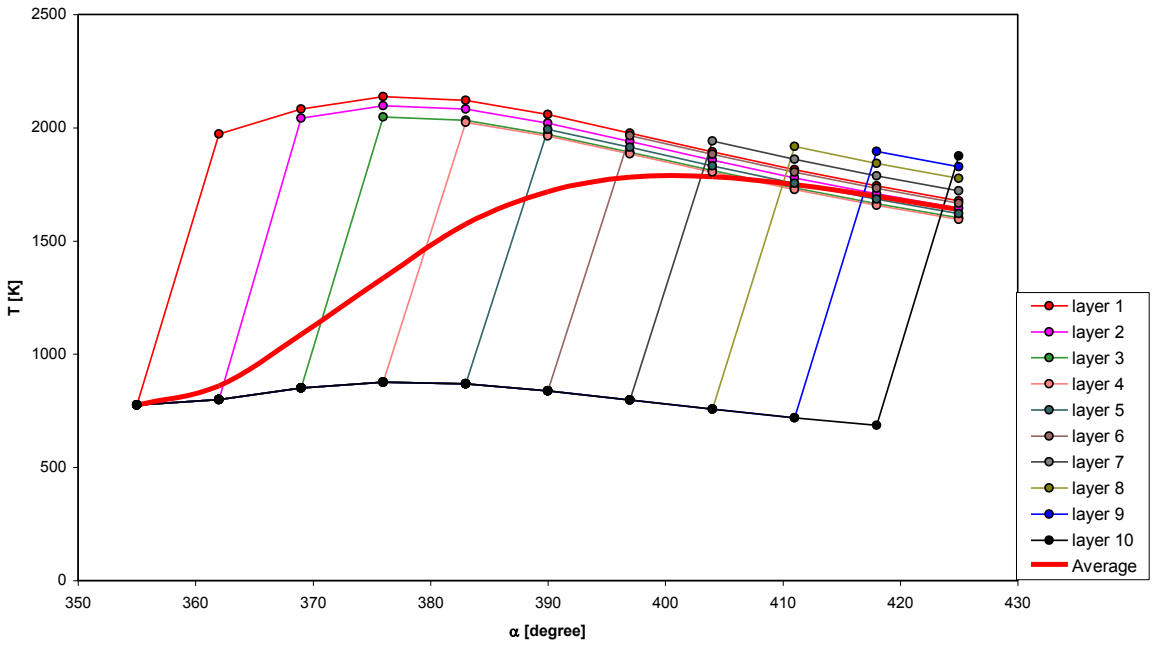


Figure 1: The courses of temperature in separated (speculated) layers of the progressive burn up of the cylinder charge of SI engine with the combustion of lean mixtures [45].

The reaction speed and the concentration changes of the reactive components in system there is describe by chemical kinetics (by means of velocity constant of chemical kinetics): for reaction of oxygen and nitrogen they are this kinetic data for NO production (ki+) and for subsequent NO decomposition (ki-) they are shown at table T1.

Table T1 [46]

Reaction	Kinetics constant [$cm^3 \cdot mol^{-1} \cdot s^{-1}$]	Temperature range [K]
(1) $O+N_2 \rightarrow NO+N$	$7.6 \times 10^{13} \cdot e^{[-38000/T]}$	2000 - 5000
(-1) $N+NO \rightarrow N_2+O$	1.6×10^{13}	300 - 5000
(2) $N+O_2 \rightarrow NO+O$	$6.4 \times 10^{9} \cdot T \cdot e^{[-3150/T]}$	300 - 3000
(-2) $O+NO \rightarrow O_2+N$	$1.5 \times 10^{9} \cdot T \cdot e^{[-19500/T]}$	1000 - 3000
(3) $N+OH \rightarrow NO+H$	4.1×10^{13}	300 - 2500
(-3) $H+NO \rightarrow OH+N$	$2.0 \times 10^{14} \cdot e^{[-23650/T]}$	2200 - 4500

By using equations 1 to 3 and kinetics constant it is possible to write the kinetics model for the rate of reactions and the rate of the time increasing of NO concentration.

$$\frac{\mathbf{d}[\mathbf{NO}]}{\mathbf{dt}} = \mathbf{k}_1^{+}[\mathbf{O}][\mathbf{N}_2] + \mathbf{k}_2^{+}[\mathbf{N}][\mathbf{O}_2] + \mathbf{k}_3^{+}[\mathbf{N}][\mathbf{OH}] - \mathbf{k}_1^{-}[\mathbf{NO}][\mathbf{N}] - \mathbf{k}_2^{-}[\mathbf{NO}][\mathbf{O}] - \mathbf{k}_3^{-}[\mathbf{NO}][\mathbf{H}], \quad (4)$$

where: [x] - concentration of individual components. [mol/cm^3]

The similar relation can be written for the rate of increasing of the atomic N concentration:

$$\frac{\mathbf{d}[\mathbf{N}]}{\mathbf{dt}} = \mathbf{k}_1^{+}[\mathbf{O}][\mathbf{N}_2] - \mathbf{k}_2^{+}[\mathbf{N}][\mathbf{O}_2] - \mathbf{k}_3^{+}[\mathbf{N}][\mathbf{OH}] - \mathbf{k}_1^{-}[\mathbf{NO}][\mathbf{N}] + \mathbf{k}_2^{-}[\mathbf{NO}][\mathbf{O}] + \mathbf{k}_3^{-}[\mathbf{NO}][\mathbf{H}]. \quad (5)$$

The change of [N] concentration in the system it is relative very little, because [N] is very reactive chemical radical. For the steady state condition there has the left side of the equation (5) the zero value (in practice effect). From the right side of the equation (5) so can be the expression of the [N] component concentration and subsequently insert to relation (4). The equation (4) so can be written to the form:

$$\frac{\mathbf{d}[\mathbf{NO}]}{\mathbf{dt}} = 2\mathbf{k}_1^{+}[\mathbf{O}][\mathbf{N}_2]\frac{1 - [\mathbf{NO}]^2/(\mathbf{K}[\mathbf{O}_2][\mathbf{N}_2])}{1 + \mathbf{k}_1^{-}[\mathbf{NO}]/(\mathbf{k}_2^{+}[\mathbf{O}_2] + \mathbf{k}_3^{+}[\mathbf{OH}])}, \quad (6)$$

where: $\mathbf{K} = (\mathbf{k}_1^{+}/\mathbf{k}_1^{-})(\mathbf{k}_2^{+}/\mathbf{k}_2^{-})$.

The radical irreversible reactions (1, 2, 3) they create the steady state very quickly with the approximately balanced of concentration of O, O_2, OH, H a N_2, which corresponds to the temperature in the system. The equilibrium rate of these reactions there is written by equation

$$\mathbf{R}_1 = \mathbf{k}_1^{+}[\mathbf{O}]_\mathbf{e}[\mathbf{N}_2]_\mathbf{e} = \mathbf{k}_1^{-}[\mathbf{NO}]_\mathbf{e}[\mathbf{N}]_\mathbf{e},$$

where $[X_i]_e$ represents the equilibrium concentration according to equation (1). Similarly

$$\mathbf{R}_2 = \mathbf{k}_2^{+}[\mathbf{N}]_\mathbf{e}[\mathbf{O}_2]_\mathbf{e} = \mathbf{k}_2^{-}[\mathbf{NO}]_\mathbf{e}[\mathbf{O}]_\mathbf{e}$$

and $$\mathbf{R}_3 = \mathbf{k}_3^{+}[\mathbf{N}]_\mathbf{e}[\mathbf{OH}]_\mathbf{e} = \mathbf{k}_3^{-}[\mathbf{NO}]_\mathbf{e}[\mathbf{H}]_\mathbf{e}$$

for equations (2) a (3). After insert of $[O]_e$, $[O_2]_e$, $[OH]_e$, $[H]_e$ a $[N_2]_e$ in place of [O], $[O_2]$, [OH], [H] a $[N_2]$ to the equation (6) and after the next make-up of this equation it will be the new form of the equation for NO production

$$\frac{\mathbf{d}[\mathbf{NO}]}{\mathbf{dt}} = \frac{2\mathbf{R}_1\left\{1 - ([\mathbf{NO}]/[\mathbf{NO}]_\mathbf{e})^2\right\}}{1 + ([\mathbf{NO}]/[\mathbf{NO}_\mathbf{e}])\mathbf{R}_1/(\mathbf{R}_2 + \mathbf{R}_3)}. \quad (7)$$

On the assumption that the relation $[NO]/[NO]_e$ is the much lower than 1 (the concentration of [NO] is significantly lower than the concentration of $[NO]_e$ for steady state condition – this approximation is good fulfillments at the start of NO creating), the relation (7) is possible write to form

$$\frac{\mathbf{d}[\mathbf{NO}]}{\mathbf{dt}} = 2\mathbf{R}_1 = 2\mathbf{k}_1^{+}[\mathbf{O}]_\mathbf{e}[\mathbf{N}_2]_\mathbf{e} \ . \tag{8}$$

The equilibrium concentration of atomic oxygen, which forms by the decomposition according to scheme $\frac{1}{2}\mathbf{O}_2 = \mathbf{O}$, there is determined by equilibrium constant (the factor RT is the recomputation between standard state at the unit of molar concentration and common standard state at the molar ratio):

$$K_{p(O)} = \frac{[O]_e (\mathbf{RT})^{0.5}}{[O_2]_e^{0.5}} \qquad \Rightarrow \qquad [O]_e = \frac{K_{p(O)}[O_2]_e^{0.5}}{(\mathbf{RT})^{0.5}} \tag{9}$$

where: R – molar (universal) gas constant [$J \cdot K^{-1} \cdot mol^{-1}$]
$K_p(O)$ - equilibrium constant for the reaction [$bar^{0.5}$]

$K_p(O)$ is determined by the empirical relation

$$\mathbf{K_{p(O)}} = 3.6 \cdot 10^3 \cdot \mathbf{e}^{\left(\frac{-31090}{\mathbf{T}}\right)} \ [bar^{0.5}] \tag{10}$$

The production of NO on the time dependence may be written by resultant relation, which is creates by combination the equations 8, 9 a 10 and using of kinetic constant k_1^{+} from tab. T1:

$$\frac{\mathbf{d}[\mathbf{NO}]}{\mathbf{dt}} = \frac{6 \cdot 10^{16}}{\mathbf{T}^{0.5}} \mathbf{e}^{\frac{-69090}{\mathbf{T}}} \cdot [\mathbf{O}_2]_\mathbf{e}^{0.5}[\mathbf{N}_2]_\mathbf{e} \qquad \left[\mathbf{mol} \cdot \mathbf{cm}^{-3} \cdot \mathbf{s}^{-1}\right] \ . \tag{11}$$

At equation (11) there are 3 quantities, which determine the created quantum of the dioxide nitrogen NO: actual middle local temperature of exhaust gas T and the local concentration of O_2 and N_2 in the elementary volume (layer). The middle temperature T of the individual volume (each) layer there is determined by the thermodynamic calculation, than for each layer must be determined the concentration of O_2 and N_2. The determination of O_2 a N_2 concentration is determined by step-by step calculation for each layer from start of the layer burning up to total end of burning in cylinder charge. The concentration of O_2 in the exhaust gas for 1st calculation step (for each layer after its burning-up) there is determined by relation:

$$[O_2]_e = \frac{M_{O_2-SP}}{M_{O2} \cdot V_i \cdot 1000} \qquad [mol \cdot cm^{-3}] \qquad (12)$$

where: $[O_2]_e$ – concentration of O_2 in exhaust gas [mol · cm^{-3}]
M_{O2-SP} – mass of residual O_2 in exhaust gas [g]
V_i – volume of ith layer after burning [dm^3]
M_{O2} – molar mass of O_2 (M_{O2} = 32 g · mol^{-1})
1000 – conversion factor from dm^3 to cm^3

The concentration of N_2 in exhaust gas for 1st calculation step of each layer after burning-up there is determined by similar method.

Its stand to reason, that the mass quantities of O_2 a N_2 in the product of burning at each layers immediately after burning-up of mixture it is determined by the total mass of the mixture in layer and by the richness of mixture (and by the chemical efficiency also). The values of these quantities (except of chemical efficiency) they are deducted from the input parameters for calculation of engine working cycle. The distribution of total mass of cylinder charge there is determined according to Wiebe equation for burning. The changes of layers volumes are induced by the change of whole volume in the cylinder according to piston motion and these changes influence the concentration of O_2 a N_2 at unit [mol · cm^{-3}] in the individual layers. At all layers there are always the same pressure values, according to course of pressure in cylinder charge.

The changes of concentration of O_2 there influence also the decrease of O_2, which was consumed for the creation of NO in the each layer. For (nth) step of the calculation there is needed to complete the balance of O_2 consumption for creation of NO at all foregoing computational steps. These is expressed by relation

$$[O_2]_{e,n} = \frac{M_{O_2-SP} - 1/2 M_{O2} \cdot V_{i,n} \cdot 1000 \cdot [NO]_{n-1}}{M_{O2} \cdot V_{i,n} \cdot 1000} \qquad [mol \cdot cm^{-3}] \ , \qquad (13)$$

where $[NO]_{n-1}$ is the concentration of NO in layer after (n-1) computational steps. The equation (12) is the special case of equation (13) for the beginning of reaction, when in the layer is not present of NO.

The computational model determines the resulting quantity of NO created in products of burning like molar concentration [mol·cm^{-3}] for each layer: summarization at the end of expansion stroke will be the total amount of NO at [mol] in the exhaust gas. The computational model compares this amount of NO to the total molar amount of exhaust gas and like the final results of calculation is the concentration of NO in exhaust gas at [ppm].

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